

10526940species

10526940aa

search claimst-3

=> fil stng

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
2.85	1166.84

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-62.40

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FILE CONTAINS CURRENT INFORMATION.  
LAST RELOADED: Feb 23, 2007 (20070223/UP).

=> fil reg

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
0.84	1167.68

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-62.40

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FILE 'REGISTRY' ENTERED AT 16:16:00 ON 01 MAR 2007  
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Property values tagged with IC are from the ZIC/VINITI data file  
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STRUCTURE FILE UPDATES: 28 FEB 2007 HIGHEST RN 923894-67-1  
DICTIONARY FILE UPDATES: 28 FEB 2007 HIGHEST RN 923894-67-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when  
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REGISTRY includes numerically searchable data for experimental and  
predicted properties as well as tags indicating availability of  
experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

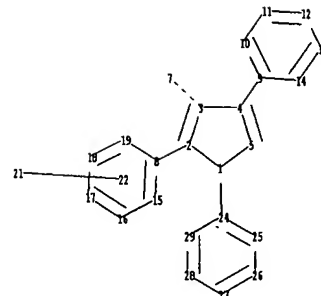
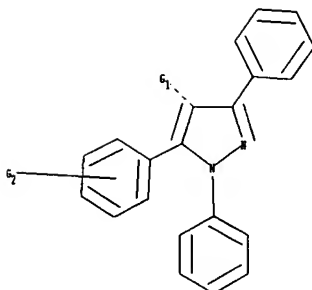
<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10526940notspec.str

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chain nodes :

7 21

ring nodes :

1 2 3 4 5 8 9 10 11 12 13 14 15 16 17 18 19 24 25 26 27 28 29

chain bonds :

1-24 2-8 3-7 4-9

ring bonds :

1-2 1-5 2-3 3-4 4-5 8-15 8-19 9-10 9-14 10-11 11-12 12-13 13-14 15-16  
16-17 17-18 18-19 24-25 24-29 25-26 26-27 27-28 28-29

exact/norm bonds :

1-2 1-5 1-24 3-7 4-5

exact bonds :

2-3 2-8 3-4 4-9

normalized bonds :

8-15 8-19 9-10 9-14 10-11 11-12 12-13 13-14 15-16 16-17 17-18 18-19  
24-25 24-29 25-26 26-27 27-28 28-29

isolated ring systems :

containing 1 : 8 : 9 :

G1:H,CH3

G2:CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:CLASS 8:Atom 9:Atom 10:Atom 11:Atom  
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 21:CLASS  
22:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom

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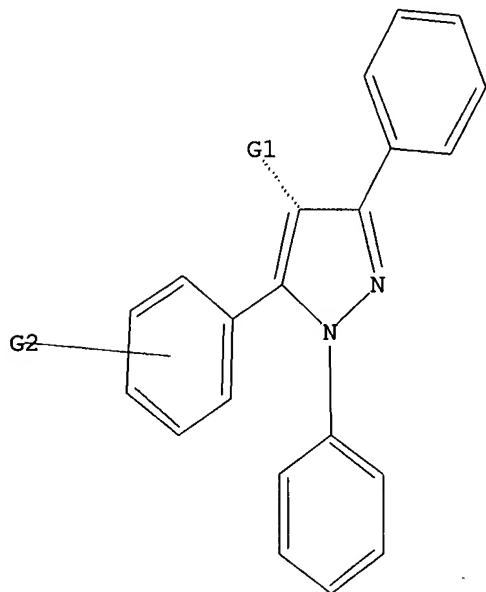
10526940species

L23 STRUCTURE UPLOADED

=> d

L23 HAS NO ANSWERS

L23 STR



G1 H, Me

G2 Me, Et, n-Pr, i-Pr, n-Bu, i-Bu, s-Bu, t-Bu

Structure attributes must be viewed using STN Express query preparation.

=> d his

(FILE 'HOME' ENTERED AT 15:24:30 ON 01 MAR 2007)

FILE 'REGISTRY' ENTERED AT 15:24:37 ON 01 MAR 2007

L1 STRUCTURE UPLOADED

L2 49 S L1

L3 11773 S L1 FULL

L4 STRUCTURE UPLOADED

L5 580 S L4 FULL SUB=L3

FILE 'CAPLUS' ENTERED AT 15:26:43 ON 01 MAR 2007

L6 470 S L5

L7 STRUCTURE UPLOADED

L8 2416251 S D

FILE 'REGISTRY' ENTERED AT 15:28:43 ON 01 MAR 2007

L9 0 S L7 SUB=L5 FULL

L10 0 S L7 FULL SUB=L3

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L14 55 S L13 FULL

FILE 'CAPLUS' ENTERED AT 15:32:16 ON 01 MAR 2007  
L15 27 S L14

FILE 'REGISTRY' ENTERED AT 15:33:56 ON 01 MAR 2007  
L16 STRUCTURE UPLOADED  
L17 8423 S L16 FULL SUB=L3

FILE 'REGISTRY' ENTERED AT 15:50:55 ON 01 MAR 2007  
L18 STRUCTURE UPLOADED  
L19 38 S L18  
L20 2044 S L18 FULL

FILE 'CAPLUS' ENTERED AT 15:51:22 ON 01 MAR 2007  
L21 111 S L20

FILE 'STNGUIDE' ENTERED AT 15:52:00 ON 01 MAR 2007

FILE 'REGISTRY' ENTERED AT 16:06:16 ON 01 MAR 2007  
L22 1 S 178625-21-3/RN

FILE 'STNGUIDE' ENTERED AT 16:07:25 ON 01 MAR 2007

FILE 'REGISTRY' ENTERED AT 16:16:00 ON 01 MAR 2007  
L23 STRUCTURE UPLOADED  
L24 1636 S L23 FULL SUB=L20

=> d 120 not 124

L24 IS NOT VALID HERE

For an explanation, enter "HELP DISPLAY".

=> s 120 not 124

L25 408 L20 NOT L24

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
44.70	1212.38

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-62.40

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FILE 'CAPLUS' ENTERED AT 16:21:14 ON 01 MAR 2007

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=> s 125

L26            56 L25

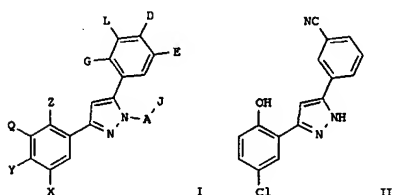
=> d ibib abs hitstr tot

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## 10526940species

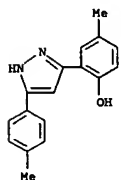
L26 ANSWER 1 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2006:1095978 CAPLUS  
DOCUMENT NUMBER: 145:438611  
TITLE: Preparation of 3,5-diphenylpyrazoles as antitumor agents  
INVENTOR(S): Kuroiwa, Shunsuke; Maruyama, Sakiko; Suzuki, Yoshihazu; Yamazaki, Hiroko  
PATENT ASSIGNEE(S): Nippon Kayaku Kabushiki Kaisha, Japan  
SOURCE: PCT Int. Appl., 45pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006109680	A1	20061019	WO 2006-JP307346	20060406
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
PRIORITY APPLN. INFO.:		JP 2005-110717		A 20050407
OTHER SOURCE(S):		HARPAT 145:438611		
GI				

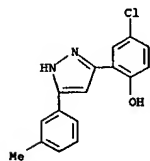


AB Title compds. I [wherein A = H, carbonyl or sulfonyl; J = (un)substituted alkyl or amino; G, Z = H, OH, alkoxy, etc.; D, E, L, Q, X, Y = H, (un)substituted aminocarbonyl, alkoxy, etc.; D and L and Q and Y may link together to form a N/S-heterocyclyl ring, with limitations] and

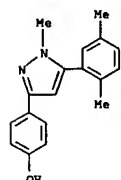
L26 ANSWER 1 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 912967-83-0 CAPLUS  
CN Phenol, 4-chloro-2-[5-(3-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



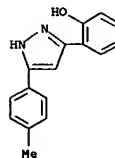
IT 362006-35-7P  
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
(reference; preparation of diphenylpyrazoles as antitumor agents)  
RN 362006-35-7 CAPLUS  
CN Phenol, 4-[5-(2,5-dimethylphenyl)-1-methyl-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



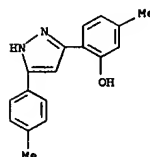
REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS

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L26 ANSWER 1 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
pharmaceutically acceptable salts thereof were prepd. as anticancer agents. For instance, treatment of 5'-chloro-2'-hydroxyacetophenone with 3-cyanobenzoyl chloride followed by cyclization with hydrazine hydrate gave diphenylpyrazole II. This product showed cell growth inhibition with IC50 of 0.23 µg/mL against MCF-7 cells and 0.066 µg/mL against MDA-MB-453 cells, resp. Therefore, the invented compds. and their pharmaceutical compns. are useful for the treatment of various cancer, such as breast cancer and lung cancer.  
IT 384352-30-1P 416877-12-8P 416880-94-9P  
912967-83-0P  
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(drug candidate; preparation of diphenylpyrazoles as antitumor agents)  
RN 384352-30-1 CAPLUS  
CN Phenol, 2-[5-(4-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



RN 416877-12-8 CAPLUS  
CN Phenol, 5-methyl-2-[5-(4-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



RN 416880-94-9 CAPLUS  
CN Phenol, 4-methyl-2-[5-(4-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

L26 ANSWER 1 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

## 10526940species

L26 ANSWER 2 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:660707 CAPLUS

DOCUMENT NUMBER: 145:292939

TITLE: Reaction of N-Monosubstituted Hydrazones with Nitroolefins: A Novel Regioselective Pyrazole Synthesis

AUTHOR(S): Deng, Xiaohu; Mani, Neelakandha S.

CORPORATE SOURCE: Department of Drug Discovery, Johnson &amp; Johnson Pharmaceutical R &amp; D LLC, San Diego, CA, 92121, USA

SOURCE: Organic Letters (2006), 8(16), 3505-3508

CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A novel regioselective synthesis of substituted pyrazoles from N-monosubstituted hydrazones and nitroolefins is described. The reaction is performed in a one-pot manner and the yields range from moderate to excellent. A key nitropyrazolidine intermediate is characterized and a plausible mechanism is proposed.

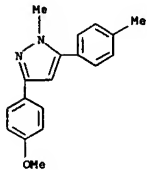
IT 908329-93-1P 908329-95-3P 908329-96-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(one-pot regioselective synthesis of substituted pyrazoles from N-monosubstituted hydrazones and nitroolefins)

RN 908329-93-1 CAPLUS

CN 1H-Pyrazole, 3-(4-methoxyphenyl)-1-methyl-5-(4-methylphenyl)- (9CI) (CA INDEX NAME)

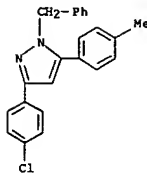


RN 908329-95-3 CAPLUS

CN 1H-Pyrazole, 3-(4-chlorophenyl)-5-(4-methylphenyl)-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

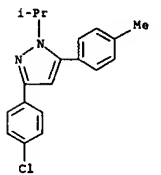
L26 ANSWER 2 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN

(Continued)



RN 908329-96-4 CAPLUS

CN 1H-Pyrazole, 3-(4-chlorophenyl)-1-(1-methylethyl)-5-(4-methylphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 40

THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 3 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:504334 CAPLUS

DOCUMENT NUMBER: 145:8083

TITLE: 1,3-Diketones from Acid Chlorides and Ketones: A Rapid and General One-Pot Synthesis of Pyrazoles

AUTHOR(S): Heller, Stephen T.; Natarajan, Svaminathan R.

CORPORATE SOURCE: Department of Medicinal Chemistry, Merck Research Laboratories, Rahway, NJ, 07065, USA

SOURCE: Organic Letters (2006), 8(13), 2675-2678

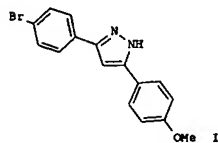
CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB 1,3-Diketones were synthesized directly from ketones and acid chlorides and were then converted in situ into pyrazoles, e.g. I, by the addition of hydrazine. This method is extremely fast, general, and chemoselective, allowing for the synthesis of previously inaccessible pyrazoles and synthetically demanding pyrazole-containing fused rings.

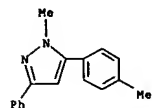
IT 66870-43-7P 888482-91-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of pyrazoles via 1,3-diketones from acid chlorides and ketones)

RN 66870-43-7 CAPLUS

CN 1H-Pyrazole, 1-methyl-5-(4-methylphenyl)-3-phenyl- (9CI) (CA INDEX NAME)

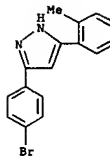


RN 888482-91-5 CAPLUS

CN 1H-Pyrazole, 3-(4-bromophenyl)-5-(2-methylphenyl)- (9CI) (CA INDEX NAME)

L26 ANSWER 3 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN

(Continued)



REFERENCE COUNT: 20

THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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## 10526940species

L26 ANSWER 4 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:473090 CAPLUS

DOCUMENT NUMBER: 145:95779

TITLE: Synthesis and molecular modelling of novel substituted-4,5-dihydro-(1H)-pyrazole derivatives as potent and highly selective monoamine oxidase-A inhibitors

AUTHOR(S): Chimentì, Franco; Bolasco, Adriana; Manna, Fedele; Secci, Daniela; Chimentì, Paola; Granese, Arianna; Befani, Olivia; Turini, Paola; Alcaro, Stefano; Ortuso, Francesco

CORPORATE SOURCE: Dipartimento di Studi di Chimica e Tecnologia delle Sostanze Biologicamente Attive, Università degli Studi di Roma "La Sapienza", Rome, 00185, Italy

SOURCE: Chemical Biology & Drug Design (2006), 67(3), 206-214

CODEN: CBDDAI; ISSN: 1747-0277

PUBLISHER: Blackwell Publishing Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 145:95779

AB This report describes novel pyrazoline derivs. investigated for their ability to selectively inhibit the activity of the A and B isoforms of monoamine oxidase. These new synthetic compds. proved to be reversible, potent, and selective inhibitors of monoamine oxidase-A rather than of monoamine oxidase-B, and are promising candidates to further advance drug discovery efforts. The most active compds. show inhibitory activity on monoamine oxidase-A in the 1.0 + 10<sup>-8</sup>-8.6 + 10<sup>-9</sup> M range.

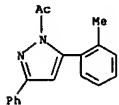
Moreover, it should be pointed out that for some compds. a high IC<sub>50</sub> ≥ 10<sup>-9</sup> M value is associated with a high A-selectivity (Selectivity Index monoamine oxidase-B/moamine oxidase-A in the 10 000-12 500 range). Further insight to understand enzyme-inhibitor mol. interaction was obtained by docking expts. with the monoamine oxidase-A and monoamine oxidase-B isoforms.

IT 895138-49-5P 895138-50-8P 895138-51-9P  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(Synthesis and mol. modeling of novel substituted-4,5-dihydro-(1H)-pyrazole derivs. as potent and highly selective monoamine oxidase-A inhibitors)

RN 895138-49-5 CAPLUS

CN 1H-Pyrazole, 1-acetyl-5-(2-methylphenyl)-3-phenyl- (9CI) (CA INDEX NAME)



RN 895138-50-8 CAPLUS

CN 1H-Pyrazole, 1-acetyl-3-(2,6-dihydroxyphenyl)-5-(2-methylphenyl)- (9CI)

L26 ANSWER 5 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:358419 CAPLUS

DOCUMENT NUMBER: 145:123923

TITLE: Correction of: 142:481542

Acylic and cyclic ureas

AUTHOR(S): Sartori, G.; Maggi, R.

CORPORATE SOURCE: Dipartimento di Chimica Organica, Industriale dell'Università, Parma, I-43100, Italy

SOURCE: Science of Synthesis (2005), 18, 665-758

CODEN: SSCYJ9

PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB A review of the preparation of cyclic and acyclic ureas.

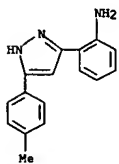
IT 178625-21-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of cyclic and acyclic ureas)

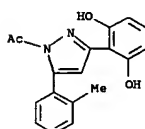
RN 178625-21-3 CAPLUS

CN Benzenamine, 2-[5-(4-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



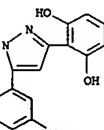
L26 ANSWER 4 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

(CA INDEX NAME)



RN 895138-51-9 CAPLUS

CN 1H-Pyrazole, 1-acetyl-3-(2,6-dihydroxyphenyl)-5-(3-methylphenyl)- (9CI)



REFERENCE COUNT: 55

THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 6 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:952848 CAPLUS

DOCUMENT NUMBER: 143:405840

TITLE: One-Pot Construction of Pyrazoles and Isoxazoles with Palladium-Catalyzed Four-Component Coupling

AUTHOR(S): Ahmed, Mohamed S. Mohamed; Kobayashi, Kei; Mori, Atsunori

CORPORATE SOURCE: Chemical Resources Laboratory, Tokyo Institute of Technology, Yokohama, 226-8503, Japan

SOURCE: Organic Letters (2005), 7(20), 4487-4489

CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 143:405840

AB Four-component coupling of a terminal alkyne, hydrazine (hydroylamine), carbon monoxide, and an aryl iodide furnishes pyrazole or isoxazole derivs. in the presence of a palladium catalyst. The reaction proceeds at room temperature and an ambient pressure of carbon monoxide in an aqueous solvent system.

IT 66870-43-7P, 1-Methyl-5-(4-methylphenyl)-3-phenyl-1H-pyrazole

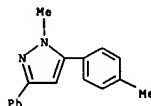
RL: SPN (Synthetic preparation); PREP (Preparation)

(one-pot construction of pyrazoles and isoxazoles by

palladium-catalyzed four-component coupling)

RN 66870-43-7 CAPLUS

CN 1H-Pyrazole, 1-methyl-5-(4-methylphenyl)-3-phenyl- (9CI) (CA INDEX NAME)



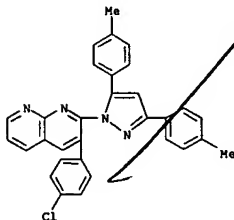
REFERENCE COUNT: 22

THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT



## 10526940species

L26 ANSWER 7 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2004:912268 CAPLUS  
DOCUMENT NUMBER: 142:316748  
TITLE: Hypervalent iodine mediated mild and efficient oxidation of pyrazolines to pyrazoles in solid state  
AUTHOR(S): Mogillalah, K.; Reddy, G. R.  
CORPORATE SOURCE: Department of Chemistry, Kakatiya University, Warangal, 506 009, India  
SOURCE: Oxidation Communications (2004), 27(3), 668-673  
CODEN: OXODW; ISSN: 0209-4541  
PUBLISHER: SciBulCom Ltd.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 142:316748  
AB An efficient and mild method for the oxidation of pyrazolinyl-1,8-naphthyridines to pyrazolyl-1,8-naphthyridines using iodobenzene diacetate in the solid state has been described. The yields are good and purity is high. The method is preparatively convenient and useful.  
IT 848356-06-9P  
RI: SPN (Synthetic preparation); PREP (Preparation)  
(hypervalent iodine mediated mild and efficient oxidation of pyrazolines to pyrazoles in solid state)  
RN 848356-06-9 CAPLUS  
CN 1,8-Naphthyridine, 2-[3,5-bis(4-methylphenyl)-1H-pyrazol-1-yl]-3-(4-chlorophenyl)- (9CI) (CA INDEX NAME)



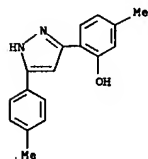
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 8 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
(un)substituted aryl, heterocyclyl, heteroaryl, cycloalkyl, alkyl, alkylcarbonyl, arylcarbonyl, heteroarylcarbonyl, heterocyclylcarbonyl, or aminocarbonyl; X = H, (un)substituted alkyl, aryl, heterocyclyl, heteroaryl, or e-substituted n-alkyl such as II are prepd. as inhibitors of ATP-binding cassette (ABC) transporters such as the cystic fibrosis transmembrane conductance regulator (CFTR) for use in the treatment of conditions such as cystic fibrosis, immunodeficiency, inflammatory disease, chronic obstructive pulmonary disease, chronic pancreatitis, or pneumonia. 4-Trifluoromethylbenzoyl chloride and 2-hydroxy-5-fluoroacetophenone are stirred in pyridine for 12 h, after which potassium hydroxide is added and the mixt. stirred for 12 h; addn. of hydrazine hydrate to a soln. of the product obtained in the first step in ethanol and heating at reflux for 3 h yields II in 30% overall yield as a yellow cryst. solid. II modulates AF508-CFTR at 275% of the effect of genistein on the same receptor. Data on the relative modulation of AF508-CFTR by some compds. of the invention as compared to genistein is provided.

IT 416877-12-8P 416880-94-9P 423735-70-0P  
423746-90-1P 423750-83-8P 423752-83-4P  
423753-85-9P 763132-75-8P 763132-82-7P  
763132-90-7P 763132-99-6P 763133-01-3P  
763133-12-6P 763133-25-1P 763133-27-3P  
763133-63-7P 763133-84-2P 763133-85-3P  
RI: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of substituted pyrazoles as modulators of ATP-binding cassette transporters such as the cystic fibrosis transmembrane conductance regulator for treatment of diseases such as cystic fibrosis, immunodeficiency, and pneumonia)

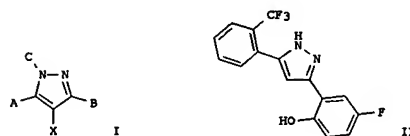
RN 416877-12-8 CAPLUS  
CN Phenol, 5-methyl-2-[5-(4-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



RN 416880-94-9 CAPLUS  
CN Phenol, 4-methyl-2-[5-(4-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

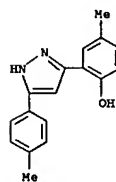
L26 ANSWER 8 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2004:780671 CAPLUS  
DOCUMENT NUMBER: 141:296010  
TITLE: Preparation of substituted pyrazoles as modulators of ATP-binding cassette transporters  
INVENTOR(S): Vangoor, Frederick F.; Hadida Ruah, Sarah S.; Singh, Ashvani K.; Olson, Eric R.; Makings, Lewis R.; Gonzalez, Jesus E., III; Rader, James A.; Chambers, Fred, III; Miller, Mark T.; Grootenhuys, Peter; Liu, Yahua  
PATENT ASSIGNEE(S): Vertex Pharmaceuticals Incorporated, USA  
SOURCE: PCT Int. Appl., 174 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004080972	A1	20040923	WO 2004-057492	20040312
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2005113423	A1	20050526	US 2004-800022	20040312
EP 1601657	A1	20051207	EP 2004-720345	20040312
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				
PRIORITY APPLN. INFO.: US 2003-453978P P 20030312				
WO 2004-057492 W 20040312				
OTHER SOURCE(S): MARPAT 141:296010				
GI				

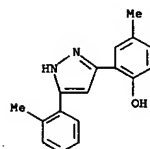


AB Pyrazoles I [A, B = (un)substituted aryl, heterocyclyl, cycloalkyl; C = H,

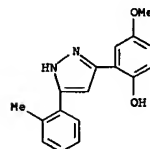
L26 ANSWER 8 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 423735-70-0 CAPLUS  
CN Phenol, 4-methyl-2-[5-(2-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



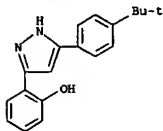
RN 423746-90-1 CAPLUS  
CN Phenol, 4-methoxy-2-[5-(2-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



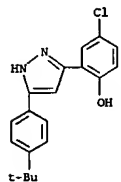
RN 423750-83-8 CAPLUS  
CN Phenol, 2-[5-(4-(1,1-dimethylethyl)phenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

# 10526940species

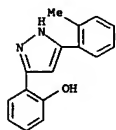
L26 ANSWER 8 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 423752-83-4 CAPLUS  
CN Phenol, 4-chloro-2-[5-[(1,1-dimethylethyl)phenyl]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

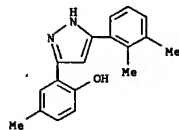


RN 423753-85-9 CAPLUS  
CN Phenol, 2-[5-(2-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

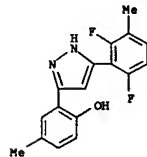


RN 763132-75-8 CAPLUS  
CN Phenol, 4-methyl-2-[5-[3-methyl-4-(trifluoromethyl)phenyl]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

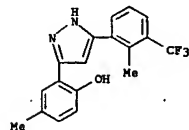
L26 ANSWER 8 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 763133-01-3 CAPLUS  
CN Phenol, 2-[5-(2,6-difluoro-3-methylphenyl)-1H-pyrazol-3-yl]-4-methyl- (9CI) (CA INDEX NAME)

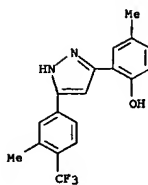


RN 763133-12-6 CAPLUS  
CN Phenol, 4-methyl-2-[5-(2-methyl-3-(trifluoromethyl)phenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

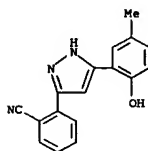


RN 763133-25-1 CAPLUS  
CN Benzenesulfonamide, N,N-diethyl-4-[5-(2-hydroxy-5-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

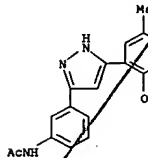
L26 ANSWER 8 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 763132-82-7 CAPLUS  
CN Benzonitrile, 2-[5-(2-hydroxy-5-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

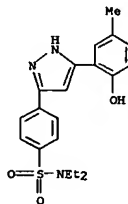


RN 763132-90-7 CAPLUS  
CN Acetamide, N-[3-[5-(2-hydroxy-5-methylphenyl)-1H-pyrazol-3-yl]phenyl]- (9CI) (CA INDEX NAME)

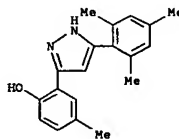


RN 763132-99-6 CAPLUS  
CN Phenol, 2-[5-(2,3-dimethylphenyl)-1H-pyrazol-3-yl]-4-methyl- (9CI) (CA INDEX NAME)

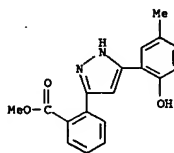
L26 ANSWER 8 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 763133-27-3 CAPLUS  
CN Phenol, 4-methyl-2-[5-(2,4,6-trimethylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



RN 763133-63-7 CAPLUS  
CN Benzoic acid, 2-[5-(2-hydroxy-5-methylphenyl)-1H-pyrazol-3-yl]-, methyl ester (9CI) (CA INDEX NAME)

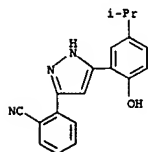


RN 763133-84-2 CAPLUS  
CN Benzonitrile, 2-[5-[2-hydroxy-5-(1-methylethyl)phenyl]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

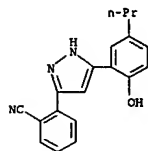
Karen Cheng

## 10526940species

L26 ANSWER 8 OF 56 CAPLUS COPYRIGHT 2007 ACS on STM (Continued)



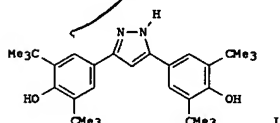
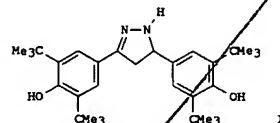
RN 763133-85-3 CAPLUS  
CN Benzonitrile, 2-[5-(2-hydroxy-5-propylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 9 OF 56 CAPLUS COPYRIGHT 2007 ACS on STM

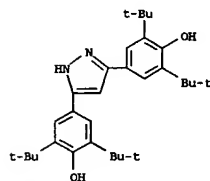
ACCESSION NUMBER: 2004:362548 CAPLUS  
DOCUMENT NUMBER: 141:106411  
TITLE: Novel 3,5-diarylpyrazolines and pyrazole as low-density lipoprotein (LDL) oxidation inhibitor  
AUTHOR(S): Jeong, Tae-Sook; Kim, Kyung Soon; Kim, Ju-Ryoung; Cho, Kyung-Hyun; Lee, Sangku; Lee, Woo Song  
CORPORATE SOURCE: National Research Laboratory of Lipid Metabolism & Atherosclerosis, Korea Research Institute of Bioscience and Biotechnology, Daejeon, 305-333, S. Korea  
SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(11), 2719-2723  
CODEN: BMCLEB; ISSN: 0960-894X  
PUBLISHER: Elsevier Science B.V.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 141:106411  
GI



AB 2,3-Diarylpyrazolines, e.g., I, and -pyrazole II were synthesized by cyclocondensation of chalcones with hydrazine, and tested for their LDL-oxidation inhibition activity. The tested compds. showed significant LDL-antioxidant activities in the TBARS assay, the lag time of conjugated diene production, the relative electrophoretic mobility (REM) of ox-LDL, the apoB-100 fragmentation, and the macrophage-mediated LDL oxidation. I and II were found to be the most active compds. as an inhibitor of LDL oxidation, and I (IC50 = 0.1 μM) was 6-fold more potent than probucol (IC50 = 0.6 μM) in the TBARS assay.  
IT 721447-01-4P  
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL

L26 ANSWER 9 OF 56 CAPLUS COPYRIGHT 2007 ACS on STM (Continued)

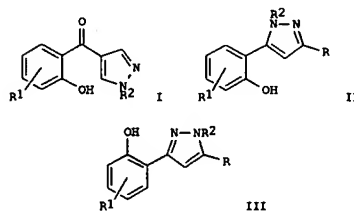
(Biological study); PREP (Preparation)  
(prepn. and low-d. lipoprotein peroxidn. inhibition of bis(di(t-butyl)hydroxyphenyl)pyrazole via oxidn. of bis(di(t-butyl)hydroxyphenyl)pyrazoline)  
RN 721447-01-4 CAPLUS  
CN Phenol, 4,4'-(1H-pyrazole-3,5-diyl)bis[2,6-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 10 OF 56 CAPLUS COPYRIGHT 2007 ACS on STM

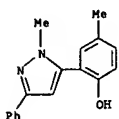
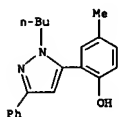
ACCESSION NUMBER: 2004:347011 CAPLUS  
DOCUMENT NUMBER: 141:332110  
TITLE: Design and synthesis of two pyrazole libraries based on o-hydroxyacetophenones  
AUTHOR(S): Borrell, Jose I.; Schuler, Elisabeth; Teixido, Jordi; Michelotti, Enrique L.  
CORPORATE SOURCE: Institut Quimic de Sarria, Grup d'Enginyeria Molecular, Universitat Ramon Llull, Barcelona, E-08017, Spain  
SOURCE: Molecular Diversity (2004), 8(2), 147-157  
CODEN: MODIF4; ISSN: 1381-1991  
PUBLISHER: Kluwer Academic Publishers  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 141:332110  
GI



AB Two new solid-phase syntheses of substituted pyrazoles are described. The first includes supporting an o-hydroxyacetophenone on Merrifield resin, Vilsmeier-Haack formulation on the Me group and cyclization with a substituted hydrazine to afford a pyrazole ring with two diversity centers, e.g. I (R1 = H, 4-F, 3,4-(MeO)2, etc.; R2 = Ph, n-Pr, 2-benzothiazolyl, etc.). The second starts from o-hydroxyacetophenone supported on Wang resin, which undergoes a Claisen condensation with a carboxylic acid ester to yield a 1,3-dicarbonyl compound that cyclizes to a pyrazole using a hydrazine, II and III (R = H, Me, Ph). Both methods have been used to synthesize two small pyrazole libraries.  
IT 771483-85-3P 771484-12-9P  
RL: CPN (Combinatorial preparation); CMBI (Combinatorial study); PREP (Preparation)  
(design and solid-phase syntheses of pyrazole libraries using o-hydroxyacetophenones, their fungicidal, insecticidal, and herbicidal activities)  
RN 771483-85-3 CAPLUS  
CN Phenol, 4-methyl-2-(1-methyl-3-phenyl-1H-pyrazol-5-yl)-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)  
CH 1  
CRN 771483-84-2

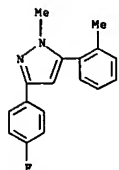
Karen Cheng

## 10526940species

L26 ANSWER 10 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
CHF C17 H16 N2 OCH 2  
CRN 76-05-1  
CHF C2 H F3 O2RN 771484-12-9 CAPLUS  
CN Phenol, 2-(1-butyl-3-phenyl-1H-pyrazol-5-yl)-4-methyl-,  
mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)CH 1  
CRN 771484-11-8  
CHF C20 H22 N2 OCH 2  
CRN 76-05-1  
CHF C2 H F3 O2

L26 ANSWER 11 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

ACCESSION NUMBER: 2004:302811 CAPLUS  
DOCUMENT NUMBER: 141:23470  
TITLE: Regioselective rapid analog syntheses of 1-methyl-3,5-diarylpyrazoles via palladium-catalyzed coupling to 3(5)-pyrazolyl nonaflates  
AUTHOR(S): Bourrain, Sylvie; Ridgill, Mark; Collins, Ian  
CORPORATE SOURCE: Department of Medicinal Chemistry, The Neuroscience Research Centre, Merck Sharp and Dohme Research Laboratories, Essex, CM20 2QR, UK  
SOURCE: Synlett (2004), (5), 795-798  
CODEN: SYNLES; ISSN: 0936-5214  
PUBLISHER: Georg Thieme Verlag  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 141:23470  
AB Regioselective rapid analog syntheses of 1-methyl-3,5-diarylpyrazoles were developed, based on Pd-catalyzed couplings to 1-methyl-3(5)-arylpyrazole nonaflates, which offered an advantage in hydrolytic stability over the corresponding triflates. The new bifunctional reagent 1-methyl-3-bromo-pyrazol-5-yl nonaflate underwent highly chemoselective Pd-catalyzed couplings to the nonaflate, followed by Suzuki couplings to the bromide, allowing sequential, regioselective introduction of the two aryl substituents.  
IT 699010-12-3P 699010-21-4P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(regioselective synthesis of 1-methyl-3,5-diarylpyrazoles through palladium-catalyzed coupling of 1-methyl-3-bromo-pyrazol-5-yl nonaflates)  
RN 699010-12-3 CAPLUS  
CN 1H-Pyrazole, 3-(4-fluorophenyl)-1-methyl-5-(2-methylphenyl)- (9CI) (CA INDEX NAME)

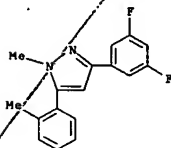
RN 699010-21-4 CAPLUS  
CN 1H-Pyrazole, 3-(3,5-difluorophenyl)-1-methyl-5-(2-methylphenyl)- (9CI)  
(CA INDEX NAME)

L26 ANSWER 10 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 11 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

## 10526940species

L26 ANSWER 12 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:211991 CAPLUS

DOCUMENT NUMBER: 140:264528

TITLE: NR3B1 nuclear receptor-binding 3-substituted pyrazole derivatives, and therapeutic uses  
 INVENTOR(S): Deuschle, Ulrich; Heck, Stefanie; Kober, Ingo; Bauer, Ulrike; Balogh, Imola  
 PATENT ASSIGNEE(S): Lion Bioscience A.-G., Germany  
 SOURCE: Eur. Pat. Appl., 45 pp.  
 CODEN: EPXOXDW

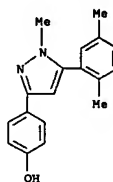
DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1398029	A1	20040317	EP 2002-20256	20020910
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
WO 2004024148	A1	20040325	WO 2003-EP7066	20030702
V: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003250877	A1	20040430	AU 2003-250877	20030702
US 2006148876	A1	20060706	US 2005-226940	20051021
PRIORITY APPLN. INFO.:			EP 2002-20256	A 20020910
			WO 2003-EP7066	W 20030702

OTHER SOURCE(S): MARPAT 140:264528  
 AB The invention discloses pyrazole derivs. which bind to the NR3B1 receptor and act as antagonists of the NR3B1 receptor. The invention further relates to the treatment of diseases and/or conditions through binding of the nuclear receptor by the compds., as well as the production of medicaments using the compds.  
 IT 362006-35-7  
 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (NR3B1 nuclear receptor-binding pyrazole derivs., and therapeutic uses)  
 RN 362006-35-7 CAPLUS  
 CN Phenol, 4-[5-(2,5-dimethylphenyl)-1-methyl-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

L26 ANSWER 12 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN

(Continued)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

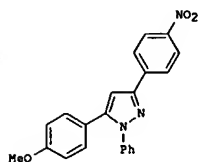
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L26 ANSWER 13 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN

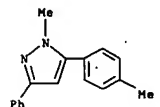
ACCESSION NUMBER: 2004:58889 CAPLUS

DOCUMENT NUMBER: 140:253486

TITLE: Regioselective synthesis of 1,3,5-substituted pyrazoles from acetylenic ketones and hydrazines  
 AUTHOR(S): Bishop, Brian C.; Brands, Karel M. J.; Gibb, Andrew D.; Kennedy, Derek J.  
 CORPORATE SOURCE: Merck Sharp & Dohme Research Laboratories, Department of Process Research, Hertfordshire, EN11 9BU, UK  
 SOURCE: Synthesis (2004), (1), 43-52  
 CODEN: SYNTRF; ISSN: 0039-7881  
 PUBLISHER: Georg Thieme Verlag  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 140:253486  
 GI



AB The synthesis of 1,3,5-trisubstituted pyrazoles, e.g., 1, from the reaction of acetylenic ketones with substituted hydrazines, is reported. The reactions were shown to be highly regioselective regardless of the nature of the substituents in the substrates and afforded essentially single pyrazole isomers in excellent yields.  
 IT 66870-43-7P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (regioselective preparation of pyrazoles via heterocyclization of diarylpropynones with hydrazines followed by dehydration)  
 RN 66870-43-7 CAPLUS  
 CN 1H-Pyrazole, 1-methyl-5-(4-methylphenyl)-3-phenyl- (9CI) (CA INDEX NAME)



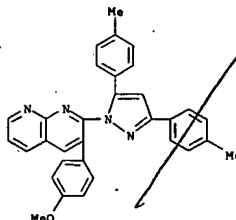
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 14 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:854945 CAPLUS

DOCUMENT NUMBER: 140:199252

TITLE: Mild and efficient oxidation of pyrazolinyl-1,8-naphthyridines to pyrazolyl-1,8-naphthyridines mediated by cerium(IV) ammonium nitrate under microwave irradiation  
 AUTHOR(S): Mogilala, K.; Reddy, N. Vasudeva; Rao, R. Babu  
 CORPORATE SOURCE: Department of Chemistry, Kakatiya University, Warangal, 506 009, India  
 SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (2003), 42B(10), 2618-2621  
 CODEN: IJSCDB; ISSN: 0376-4699  
 PUBLISHER: National Institute of Science Communication  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 140:199252  
 AB Cerium(IV) ammonium nitrate (CAN) was used as an effective oxidizing agent for the oxidation of pyrazolinyl-1,8-naphthyridines to the corresponding pyrazolyl-1,8-naphthyridines under microwave irradiation with high yields.  
 IT 663155-83-7P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (oxidation of pyrazolinyl-1,8-naphthyridines to pyrazolyl-1,8-naphthyridines using cerium(IV) ammoniumnitrate oxidant under microwave irradiation)  
 RN 663155-83-7 CAPLUS  
 CN 1,8-Naphthyridine, 2-[3,5-bis(4-methylphenyl)-1H-pyrazol-1-yl]-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

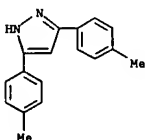


REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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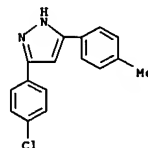
Check Dates

L26 ANSWER 15 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2002:855864 CAPLUS  
 DOCUMENT NUMBER: 139:214344  
 TITLE: Product class 1: pyrazoles  
 AUTHOR(S): Stanovnik, B.; Svete, J.  
 CORPORATE SOURCE: Faculty of Chemistry and Chemical Technology, Division of Organic Chemistry, Ljubljana, 61000, Slovenia  
 SOURCE: Science of Synthesis (2002), 12, 15-225  
 CODEN: SSCYJ9  
 PUBLISHER: Georg Thieme Verlag  
 DOCUMENT TYPE: Journal; General Review  
 LANGUAGE: English  
 AB A review. Methods for preparing pyrazoles are reviewed including cyclization, ring transformation, aromatization and substituent modifications.  
 IT 93330-77-9P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of pyrazoles via cyclization, ring transformation, aromatization and substituent modifications)  
 RN 93330-77-9 CAPLUS  
 CN 1H-Pyrazole, 3,5-bis(4-methylphenyl)- (9CI) (CA INDEX NAME)



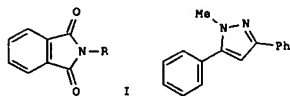
REFERENCE COUNT: 909 THERE ARE 909 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 16 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2002:150071 CAPLUS  
 DOCUMENT NUMBER: 137:33270  
 TITLE: Novel tandem reactions of 2,2'-sulfonylbis(1,3-diarylprop-2-en-1-ones) with hydrazine. Formation of 3,6-diarylpyridazines and 3,5-diarylpyrazoles  
 AUTHOR(S): Gnanadeepam, M.; Selvaraj, S.; Perumal, S.; Renuga, S.  
 CORPORATE SOURCE: Department of Chemistry, Fatima College, Madurai, 625 018, India  
 SOURCE: Tetrahedron (2002), 58(11), 2227-2230  
 CODEN: TETRA; ISSN: 0040-4020  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 137:33270  
 AB The 2,2'-sulfonylbis(1,3-diarylprop-2-en-1-ones) undergo tandem reactions with hydrazine affording 3,6-diarylpyridazines and 3,5-diarylpyrazoles unexpectedly, the latter predominating.  
 IT 131138-54-0P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of 3,6-diarylpyridazines and 3,5-diarylpyrazoles by tandem reactions of sulfonylbis(diarylpropenones) with hydrazine)  
 RN 131138-54-0 CAPLUS  
 CN 1H-Pyrazole, 3-(4-chlorophenyl)-5-(4-methylphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

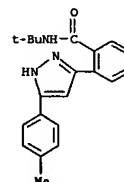
L26 ANSWER 17 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2002:71213 CAPLUS  
 DOCUMENT NUMBER: 136:401679  
 TITLE: Regioselective synthesis of pyrazoles via the ring cleavage of 3-substituted N-alkylated 3-hydroxyisoindolin-1-ones  
 AUTHOR(S): Chang, Kyu-Tae; Choi, Yong Hyun; Kim, Seung-Ho; Yoon, Yong-Jin; Lee, Woo Song  
 CORPORATE SOURCE: Proteome Research Laboratory, Korea Research Institute of Bioscience and Biotechnology, Taejeon, 305-333, S. Korea  
 SOURCE: Journal of the Chemical Society, Perkin Transactions 1 (2002), (2), 207-210  
 CODEN: JCSPCE; ISSN: 1472-7781  
 PUBLISHER: Royal Society of Chemistry  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 136:401679  
 GI



AB N-Alkyl (Me, Et, i-Pr, t-Bu)-substituted phthalimides I (R = Me, Et, i-Pr, t-Bu) were easily transformed to mono-, di-, or tri-substituted pyrazoles, e.g., II via a one-pot addition-decyclization-cyclocondensation process.  
 The regiochem. of the pyrazole ring was determined by X-ray crystallog. anal. and  
 1H NMR expts.  
 IT 431877-70-2P 431877-76-8P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of pyrazoles from N-alkylphthalimides via addition of lithium alkylacetylides, ring cleavage of intermediate N-alkylhydroxyisoindolinones and subsequent regioselective cyclocondensation with hydrazines)  
 RN 431877-70-2 CAPLUS  
 CN Benzamide, N-methyl-2-[5-(4-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

L26 ANSWER 17 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

AB  
 RN 431877-76-8 CAPLUS  
 CN Benzamide, N-(1,1-dimethylethyl)-2-[5-(4-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

102b - Claims 1, 2  
 103 - Claim 3

Karen Cheng

## 10526940species

L26 ANSWER 18 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:749722 CAPLUS

DOCUMENT NUMBER: 136:47977

TITLE:

New antimitotic agents with activity in multidrug-resistant cell lines and in vivo efficacy in murine tumor models

AUTHOR(S):

Szczepankiewicz, Bruce G.; Liu, Gang; Jia, Hwan-Soo; Tasker, Andrew S.; Gunawardana, Indrani V.; von Geldern, Thomas W.; Gwaltney, Stephen L.; Wu-Wong, J. Ruth; Gehrke, Laura; Chiou, William J.; Credo, R. Bruce; Alder, Jeffery D.; Nukkala, Michael A.; Zielinski, Nicolette A.; Jarvis, Ken; Mollison, Karl W.; Frost, David J.; Bauch, Joy L.; Hui, Yu Hua; Claiborne, Akiyo K.; Li, Qun; Rosenberg, Saul H. Pharmaceutical Products Division, Abbott Laboratories, Abbott Park, IL, 60064, USA

CORPORATE SOURCE:

SOURCE:

Journal of Medicinal Chemistry (2001), 44(25), 4416-4430

PUBLISHER:

CODEN: JMCMAH; ISSN: 0022-2623

DOCUMENT TYPE:

American Chemical Society

LANGUAGE:

Journal

OTHER SOURCE(S):

English

AB

During a screen for compds. that could inhibit cell proliferation, a series of new tubulin-binding compds. was identified with the discovery of oxadiazoline A-105972. This compound showed good cytotoxic activity against non-multi-drug-resistant and multi-drug-resistant cancer cell lines, but its utility in vivo was limited by a short half-life. Medicinal chemical efforts led to the discovery of indolyloxazoline A-259745, which maintained all of the in vitro activity seen with oxadiazoline 1, but also demonstrated a better pharmacokinetic profile, and dose-dependent in vivo activity. Over a 28 day study, indolyloxazoline A-259745 increased the life span of tumor-implanted mice by up to a factor of 3 upon oral dosing. This compound, and others of its structural class, may prove to be useful in the development of new chemotherapeutic agents to treat human cancers.

IT 380922-11-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(antimitotic agents with activity in multidrug-resistant cell lines and in vivo efficacy in murine tumor models)

RN

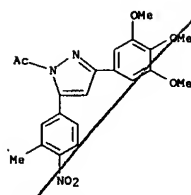
380922-11-2 CAPLUS

CN

1H-Pyrazole, 1-acetyl-5-(3-methyl-4-nitrophenyl)-3-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

L26 ANSWER 18 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN

(Continued)



REFERENCE COUNT:

14

THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

claim 1 =

L26 ANSWER 19 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:658144 CAPLUS

DOCUMENT NUMBER: 135:34441

TITLE:

Regioselective Synthesis of Polysubstituted Pyrazoles and Isoxazoles

AUTHOR(S):

Katritzky, Alan R.; Wang, Mingyi; Zhang, Suoming; Voronkov, Michael V.; Steel, Peter J.

CORPORATE SOURCE:

Department of Chemistry Center for Heterocyclic Compounds, University of Florida, Gainesville, FL, 32611-7200, USA

SOURCE:

Journal of Organic Chemistry (2001), 66(20), 6787-6791

PUBLISHER:

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE:

American Chemical Society

LANGUAGE:

Journal

OTHER SOURCE(S):

English

AB

A regioselective synthesis has been developed for the preparation of unsym. 1,3,5-triaryl-4-alkylpyrazolines and -pyrazoles by treatment of α-benzotriazolyl-α,β-unsatd. ketones with monosubstituted hydrazines followed by alkylation at the 4-position of the pyrazoline ring. Reaction of α-benzotriazolyl-α,β-unsatd. ketones with hydroxylamine gives 3,5-disubstituted isoxazoles regioselectively.

IT

66870-43-7P 371772-74-6P

RL: SPN (Synthetic preparation); PREP (Preparation)

RN

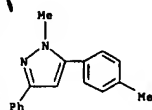
(regioselective synthesis of polysubstituted pyrazoles and isoxazoles)

CN

66870-43-7 CAPLUS

1H-Pyrazole, 1-methyl-5-(4-methylphenyl)-3-phenyl- (9CI) (CA INDEX NAME)

not subst. phenyl



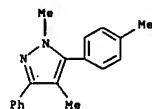
RN 371772-74-6 CAPLUS

CN

1H-Pyrazole, 1,4-dimethyl-5-(4-methylphenyl)-3-phenyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT



L26 ANSWER 20 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:553563 CAPLUS

DOCUMENT NUMBER: 133:164050

TITLE:

Preparation of diarylpyrazolocarboxylates as erythropoietin sensitizers.

INVENTOR(S):

Stoltefuss, Jürgen; Braunlich, Gabriele; Hinzen, Berthold; Kramer, Thomas; Fernerstorfer, Josef; Studemann, Thomas; Nielsch, Ulrich; Bechem, Martin; Lohmann, Emanuel; Gerdes, Christoph; Sperzel, Michael; Lustig, Klemens; Mayr, Lorenz

PATENT ASSIGNEE(S):

Bayer Aktiengesellschaft, Germany

SOURCE:

PCT Int. Appl., 38 pp.

DOCUMENT TYPE:

CODEN: PIXXD2

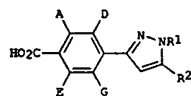
LANGUAGE:

Patent

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000046208	A1	20000810	WO 2000-EP511	20000124
V: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
DE 19904406	A1	20000810	DE 1999-19904406	19990204
CA 2361816	A1	20000810	CA 2000-2361816	20000124
EP 1150958	A1	20011107	EP 2000-910605	20000124
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002536365	T	20021029	JP 2000-597278	20000124
PRIORITY APPL. INFO.: DE 1999-19904406 A 19990204 WO 2000-EP511 W 20000124				
OTHER SOURCE(S): MARPAT 133:164050				
GI				

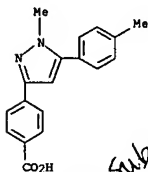


AB Title compds. [I: A, D, E, G = H, halo, CF<sub>3</sub>, OH, alkyl, alkoxy; R<sub>1</sub> = H, alkyl; R<sub>2</sub> = (substituted) naphthyl, (benzo-fused) heterocyclyl], were prepared Thus, 1-(4-methoxycarbonylphenyl)-3-(4-trifluoromethylphenyl)-1,3-propanedione was refluxed with N<sub>2</sub>H<sub>4</sub> to give 3-(4-methoxycarbonylphenyl)-5-(4-trifluoromethylphenyl)pyrazole. This was treated with NaH/MeI in THF to give 3-(4-methoxycarbonylphenyl)-1-methyl-5-(4-

Karen Cheng

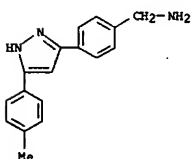
## 10526940species

L26 ANSWER 20 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
 trifluoromethylphenyl)pyrazole. This was refluxed with aq. NaOH in EtOH to give 3-(4-carboxyphenyl)-1-methyl-5-(4-trifluoromethylphenyl)pyrazole. The latter at 10  $\mu$ M gave an 86% increase in erythrocyte precursor cells.  
 IT 287951-36-4P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of diarylpyrazolecarboxylates as erythropoietin sensitizers)  
 RN 287951-36-4 CAPLUS  
 CN Benzoic acid, 4-[1-methyl-5-(4-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

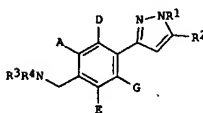
L26 ANSWER 21 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of pyrazolylbenzylamines for treatment of anemia)  
 RN 287727-26-8 CAPLUS  
 CN Benzenemethanamine, 4-[5-(4-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 21 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2000:553561 CAPLUS  
 DOCUMENT NUMBER: 133:150559  
 TITLE: Preparation of pyrazolylbenzylamines for treatment of anemia.  
 INVENTOR(S): Stoltefuss, Jurgen; Braunlich, Gabriele; Hinzen, Berthold; Kramer, Thomas; Pernerstorfer, Josef; Studemann, Thomas; Wilsch, Ulrich; Bechem, Martin; Lohrmann, Emanuel; Gerdes, Christoph; Sperzel, Michael; Lustig, Klemens; Mayr, Lorenz  
 PATENT ASSIGNEE(S): Bayer Aktiengesellschaft, Germany  
 SOURCE: PCT Int. Appl., 43 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

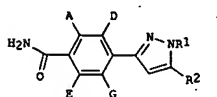
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000046206	A1	20000810	WO 2000-EP503	20000124
V: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LA, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
DE 19904396	A1	20000810	DE 1999-19904396	19990204
PRIORITY APPL. INFO.:			DE 1999-19904396	A 19990204
OTHER SOURCE(S):			MARPAT 133:150559	



AB Title compds. [I: A, D, E, G = H, halo, CF3, OH, alkyl, alkoxy; R1 = H, alkyl; R2 = (substituted) aryl, 5-6 membered (benzo-condensed) heteroaryl; R3, R4 = H, acyl, alkyl, aminocarbonyl], were prepared as erythropoietin sensitizers (no data). Thus, 3-(4-aminocarbonylphenyl)-5-(4-methoxyphenyl)-1-methylpyrazole was stirred with BH3 in THF to give 3-(4-aminomethylphenyl)-5-(4-methoxyphenyl)-1-methylpyrazole.  
 IT 287727-26-8P

L26 ANSWER 22 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2000:553561 CAPLUS  
 DOCUMENT NUMBER: 133:150559  
 TITLE: Preparation of pyrazolylarylcarboxamides for treatment of anemia.  
 INVENTOR(S): Stoltefuss, Jurgen; Braunlich, Gabriele; Hinzen, Berthold; Kramer, Thomas; Pernerstorfer, Josef; Studemann, Thomas; Wilsch, Ulrich; Bechem, Martin; Lohrmann, Emanuel; Gerdes, Christoph; Sperzel, Michael; Lustig, Klemens; Mayr, Lorenz  
 PATENT ASSIGNEE(S): Bayer Aktiengesellschaft, Germany  
 SOURCE: PCT Int. Appl., 37 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000045894	A2	20000810	WO 2000-EP519	20000124
WO 2000045894	A3	20010419		
V: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LA, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
DE 19904397	A1	20000810	DE 1999-19904397	19990204
CA 2361636	A1	20000810	CA 2000-2361636	20000124
EP 1148979	A2	20011031	EP 2000-909096	20000124
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002536348	T	20021029	JP 2000-597013	20000124
PRIORITY APPL. INFO.:			DE 1999-19904397	A 19990204
OTHER SOURCE(S):			WO 2000-EP519	W 20000124
GI			MARPAT 133:150558	

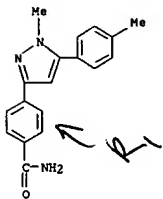


AB Use of title compds. [I: A, D, E, G = H, halo, CF3, OH, alkyl, alkoxy; R1 = H, alkyl; R2 = (substituted) aryl, 5-6 membered (benzo-condensed) heterocyclyl] as drugs for treatment of disease, particularly anemia, is claimed (no data). Acetophenone-4-carboxylic acid supported on Tentagel SAM resin was heated at 90° with Me 4-bromobenzoate and NaH in

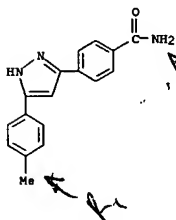
Karen Cheng



L26 ANSWER 22 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
 dimethylacetamide; the product was stirred with MeNH<sub>2</sub>H<sub>2</sub> in dimethylacetamide at 70° followed by resin cleavage with CF<sub>3</sub>CO<sub>2</sub>H in CH<sub>2</sub>Cl<sub>2</sub> to give 3-(aminocarbonylphenyl)-5-(4-bromophenyl)-1-methylpyrazole.  
 IT 287395-67-9P 287395-72-6P  
 RI: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of pyrazolylarylcarboxamides for treatment of anemia)  
 RN 287395-67-9 CAPLUS  
 CN Benzamide, 4-[1-methyl-5-(4-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



RN 287395-72-6 CAPLUS  
 CN Benzamide, 4-[5-(4-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

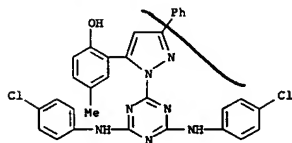


*Claims 1-3*

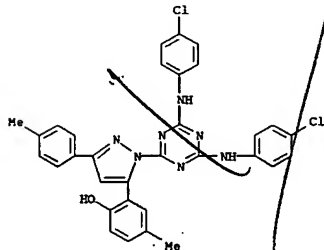
*not alkyl phenyl for R3*

*102b-claims 1-2  
103-claim 3.*

L26 ANSWER 23 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

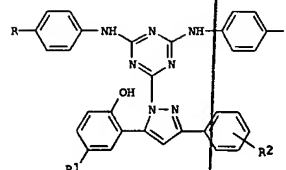


RN 321896-93-9 CAPLUS  
 CN Phenol, 2-[1-[4,6-bis[(4-chlorophenyl)amino]-1,3,5-triazin-2-yl]-3-(4-methylphenyl)-1H-pyrazol-5-yl]-4-methyl- (9CI) (CA INDEX NAME)



RN 321896-95-1 CAPLUS  
 CN Phenol, 2-[1-[4,6-bis[(4-chlorophenyl)amino]-1,3,5-triazin-2-yl]-3-(3-chlorophenyl)-1H-pyrazol-5-yl]-4-methyl- (9CI) (CA INDEX NAME)

L26 ANSWER 23 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2000:545310 CAPLUS  
 DOCUMENT NUMBER: 134:131499  
 TITLE: Synthesis and biological activity of 2,4-bis(substituted anilino)-6-(pyrazolyl)-s-triazines  
 AUTHOR(S): Manoj D. V.; Chavan, V. P.; Mane, A. S.; Bhavsar, S. B.; Shingare, M. S.  
 CORPORATE SOURCE: P.Q. Dept. of Chemistry S.C.S. College, Dr. B.A. Marathwada University, Aurangabad, 431 004, India  
 SOURCE: Indian Journal of Heterocyclic Chemistry (2000), 9(4), 27-274  
 CODEN: IJCHEI; ISSN: 0971-1627  
 PUBLISHER: Prof. R. S. Varma  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 134:131499  
 GI

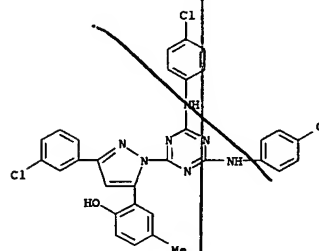


AB Title compds. such as I (R = Cl, NO<sub>2</sub>, Me, EtO; R1 = Me, Cl; R2 = H, 4-Me, 4-OMe, 3-Cl, 4-NO<sub>2</sub>) were prepared. These compds. possessed promising antibacterial and antifungal activities.

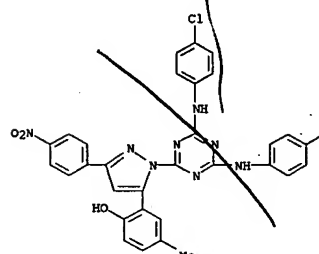
IT 321896-92-8P 321896-93-9P 321896-95-1P  
 321896-96-2P 321897-05-6P 321897-06-7P  
 321897-07-8P 321897-14-7P 321897-15-8P  
 321897-16-9P 321897-17-0P  
 RI: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
 (2,4-bis(substituted anilino)-6-(pyrazolyl)-s-triazines and their antimicrobial activity)

RN 321896-92-8 CAPLUS  
 CN Phenol, 2-[1-[4,6-bis[(4-chlorophenyl)amino]-1,3,5-triazin-2-yl]-3-(4-methylphenyl)-1H-pyrazol-5-yl]-4-methyl- (9CI) (CA INDEX NAME)

L26 ANSWER 23 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



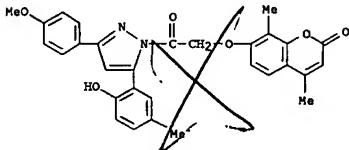
RN 321896-96-2 CAPLUS  
 CN Phenol, 2-[1-[4,6-bis[(4-chlorophenyl)amino]-1,3,5-triazin-2-yl]-3-(4-nitrophenyl)-1H-pyrazol-5-yl]-4-methyl- (9CI) (CA INDEX NAME)



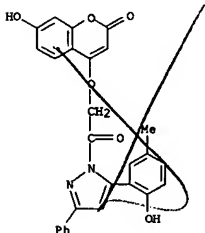
RN 321897-05-6 CAPLUS  
 CN Phenol, 2-[1-[4,6-bis[(4-nitrophenyl)amino]-1,3,5-triazin-2-yl]-3-(4-methoxyphenyl)-1H-pyrazol-5-yl]-4-methyl- (9CI) (CA INDEX NAME)

## 10526940species

L26 ANSWER 24 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

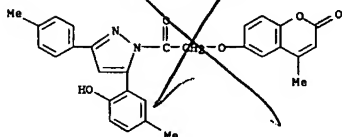


RN 263407-72-3 CAPLUS  
CN 1H-Pyrazole, 5-(2-hydroxy-5-methylphenyl)-1-[[[(7-hydroxy-2-oxo-2H-1-benzopyran-4-yl)oxy]acetyl]-3-phenyl- (9CI) (CA INDEX NAME)

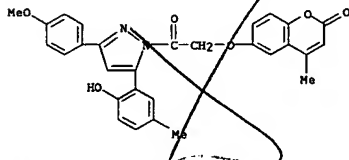


RN 263407-73-4 CAPLUS  
CN 1H-Pyrazole, 5-(2-hydroxy-5-methylphenyl)-1-[[[(7-hydroxy-2-oxo-2H-1-benzopyran-4-yl)oxy]acetyl]-3-(4-methylphenyl)- (9CI) (CA INDEX NAME)

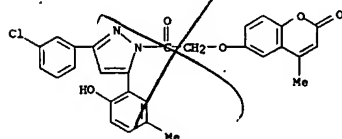
L26 ANSWER 24 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 263407-82-5 CAPLUS  
CN 1H-Pyrazole, 5-(2-hydroxy-5-methylphenyl)-3-(4-methoxyphenyl)-1-[[[(4-methyl-2-oxo-2H-1-benzopyran-6-yl)oxy]acetyl]- (9CI) (CA INDEX NAME)



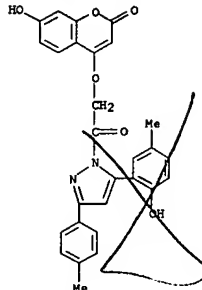
RN 263407-83-6 CAPLUS  
CN 1H-Pyrazole, 3-(3-chlorophenyl)-5-(2-hydroxy-5-methylphenyl)-1-[[[(4-methyl-2-oxo-2H-1-benzopyran-6-yl)oxy]acetyl]- (9CI) (CA INDEX NAME)



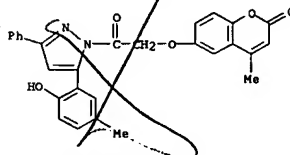
REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Karen Cheng

L26 ANSWER 24 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 263407-80-3 CAPLUS  
CN 1H-Pyrazole, 5-(2-hydroxy-5-methylphenyl)-1-[[[(4-methyl-2-oxo-2H-1-benzopyran-6-yl)oxy]acetyl]-3-phenyl- (9CI) (CA INDEX NAME)



RN 263407-81-4 CAPLUS  
CN 1H-Pyrazole, 5-(2-hydroxy-5-methylphenyl)-1-[[[(4-methyl-2-oxo-2H-1-benzopyran-6-yl)oxy]acetyl]-3-(4-methylphenyl)- (9CI) (CA INDEX NAME)

L26 ANSWER 25 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:526163 CAPLUS

DOCUMENT NUMBER: 131:286138

TITLE:

A new series of proton/charge transfer molecules: synthesis and spectral studies of 2-(5-aryl-1-carbomethoxy-1H-pyrazol-3-yl)phenols

AUTHOR(S):

Rampy, Mary E.; Halkyard, Carrie E.; Williams, Angela R.; Angel, April J.; Hurst, Douglas R.; Townsend, Jessica D.; Finsfrock, Anne E.; Beam, Charles F.; Studer-Martinez, Shannon L.

CORPORATE SOURCE:

Department of Chemistry and Biochemistry, College of Charleston, Charleston, SC, 29424, USA

SOURCE:

Photochemistry and Photobiology (1999), 70(2), 176-183

CODEN: PHCBAP; ISSN: 0031-8655

PUBLISHER:

American Society for Photobiology

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB

The carbomethoxyhydrazones of 2'-hydroxyacetophenone was trilitiated with excess lithium diisopropylamide and C-acylated with a variety of benzoate esters followed by acid cyclization of the intermediates to 2-(5-aryl-1-carbomethoxy-1H-pyrazol-3-yl)phenols [3-(2-hydroxyphenyl)-1H-pyrazoles]. The products were characterized by Fourier transform-IR, 1H NMR, 13C NMR, UV-visible absorption and fluorescence. All the derivs in n-heptane have an absorption maximum at .apprx.304 nm and an extremely weak (Φ<sub>f</sub> = 10<sup>-4</sup>) fluorescence with maxima in the range of 335-460 nm. The broad range of fluorescence maxima and fluorescence quantum yields is attributed to varying contributions of charge transfer that are dependent on both the identity of the substituent and solvent polarity. A phenomenally large Stokes-shifted fluorescence maximum at 620 nm was observed

for 2-(1-carbomethoxy-5-[4-(dimethylaminophenyl)]-1H-pyrazol-3-yl)phenol in n-heptane and attributed to excited-state intramol. proton transfer. As a result, competitive excited-state proton/charge transfer properties have been observed in the pyrazoles studied, of which the spectral properties can be fine tuned by substituent as well as solvent effects.

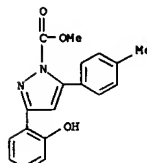
IT

246229-49-2P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (synthesis and evaluation of excited-state charge transfer and proton transfer in 2-(5-aryl-1-carbomethoxy-1H-pyrazol-3-yl)phenols)

RN 246229-49-2 CAPLUS

CN 1H-Pyrazole-1-carboxylic acid, 3-(2-hydroxyphenyl)-5-(4-methylphenyl)-, methyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT:

41

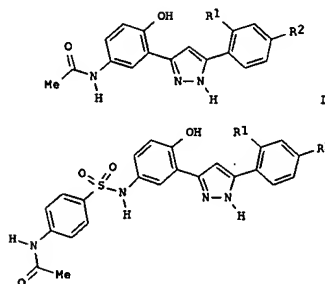
THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

C, to Cg:  
R2 = subst. acyl  
claim 1

L26 ANSWER 25 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

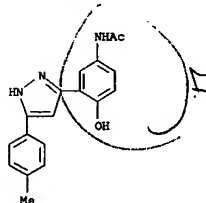
L26 ANSWER 26 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN

1999:440556 CAPLUS  
 131:271831  
 TITLE: Synthesis of some new 3,5-diarylpyrazoles and their antibacterial activity  
 AUTHOR(S): Falker, R. B.; Master, H. E.  
 CORPORATE SOURCE: Nadkarny Sacasa Research Laboratory, Department of Chemistry, St. Xavier's College, Mumbai, 400 001, India  
 SOURCE: Indian Journal of Heterocyclic Chemistry (1999), 8(4), 315-318  
 CODEN: IJCHEI; ISSN: 0971-1627  
 PUBLISHER: Prof. R. S. Varma  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

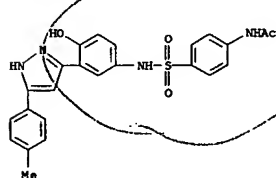


AB 3-(5-Acetamido-2'-hydroxyphenyl)-5-aryl-1H-pyrazoles I (R<sup>1</sup> = H, Cl; R<sup>2</sup> = H, Me, Cl) were synthesized from 3-(2'-hydroxyphenyl)-5'-aryl-1,3-diketones and 6-acetamidoflavones resp. which on hydrolysis gave the corresponding 5'-amino-2'-hydroxyphenylpyrazole hydrochlorides. Condensation of 5'-amino-2'-hydroxyphenylpyrazole hydrochlorides with p-acetamidobenzenesulfonyl chloride in pyridine gave 3-(5'-acetamidobenzenesulfonylphenyl)-5-arylpyrazoles II. I and II have been screened for antimicrobial activity against gram-pos. and gram-neg. bacteria.  
 IT 245468-37-5P 245468-46-6P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent) (preparation of 3,5-diarylpyrazoles and their antibacterial activity)  
 RN 245468-37-5 CAPLUS

L26 ANSWER 26 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
 CN Acetamide, N-[4-[[[4-hydroxy-3-[5-(4-methylphenyl)-1H-pyrazol-3-yl]phenyl]amino]sulfonyl]phenyl]- (9CI) (CA INDEX NAME)

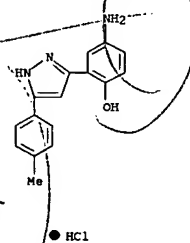


RN 245468-46-6 CAPLUS  
 CN Acetamide, N-[4-[[[4-hydroxy-3-[5-(4-methylphenyl)-1H-pyrazol-3-yl]phenyl]amino]sulfonyl]phenyl]- (9CI) (CA INDEX NAME)

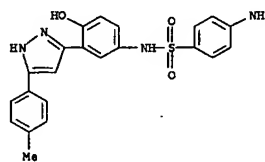


IT 245468-42-2P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of 3,5-diarylpyrazoles and their antibacterial activity)  
 RN 245468-42-2 CAPLUS  
 CN Phenol, 4-amino-2-[5-(4-methylphenyl)-1H-pyrazol-3-yl]-, monohydrochloride (9CI) (CA INDEX NAME)

L26 ANSWER 26 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



IT 245468-50-2P  
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of 3,5-diarylpyrazoles and their antibacterial activity)  
 RN 245468-50-2 CAPLUS  
 CN Benzenesulfonamide, 4-amino-N-[4-hydroxy-3-[5-(4-methylphenyl)-1H-pyrazol-3-yl]phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

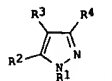
## 10526940species

L26 ANSWER 29 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1996:616374 CAPLUS  
 DOCUMENT NUMBER: 125:247813  
 TITLE: Process for preparation of N-substituted pyrazoles.  
 INVENTOR(S): Merkle, Hans Rupert; Fretschner, Erich; Schroeder, Juergen  
 PATENT ASSIGNEE(S): BASF A.-G., Germany  
 SOURCE: Ger. Offen., 7 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 3  
 PATENT INFORMATION:

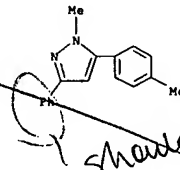
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19509958	A1	19960919	DE 1995-19509958	19950318
CA 2213853	A1	19960912	CA 1996-2213853	19960227
WO 9627589	A1	19960912	WO 1996-EP790	19960227
W: AU, BG, BR, CA, CN, CZ, FI, HU, JP, KR, MX, NO, NZ, PL, SG, SK, TR, UA, US, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9649418	A	19960923	AU 1996-49418	19960227
AU 698827	B2	19980405		
EP 813526	A1	19971129	EP 1996-905803	19960227
EP 813526	B1	20040204		
R: AT, BE, CH, DE, ES, FR, GB, IT, LI, NL				
CN 1177348	A	19980325	CN 1996-192351	19960227
CN 1070479	B	20010905		
BR 9607649	A	19980616	BR 1996-7649	19960227
HU 9801876	A2	19981130	HU 1998-1876	19960227
HU 221418	B1	20020928		
JP 11501040	T	19990126	JP 1996-526574	19960227
PL 183813	B1	20020731	PL 1996-322114	19960227
AT 258922	T	20040215	AT 1996-905803	19960227
ES 2216045	T3	20041016	ES 1996-905803	19960227
IL 117290	A	20010111	IL 1996-117290	19960228
US 5840913	A	19981124	US 1997-913177	19970820
FI 9703592	A	19970903	FI 1997-3592	19970903
NO 9704044	A	19970903	NO 1997-4044	19970903
NO 307882	B1	20000613		
BG 63304	B1	20010928	BG 1997-101908	19970924
PRIORITY APPLN. INFO.:				
DE 1995-19507600 A 19950304				
DE 1995-19507699 A 19950304				
DE 1995-19509361 A 19950315				
DE 1995-19509958 A 19950318				
WO 1996-EP790 W 19960227				

OTHER SOURCE(S): CASREACT 125:247813; MARPAT 125:247813  
 GI

L26 ANSWER 29 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



AB N-Substituted Pyrazoles I [R1 = C1-12 alkyl, C7-20 phenylalkyl; R2, R3, R4 = H, C1-12, C7-20 alkyl, (un)substituted aryl] are prepared by liquid-phase alkylation of pyrazoles I [R1 = H] with an alc./ester R1OR5 [R1 as above; R5 = H or COR1] at 50-400° and 0.001-100 bar, in the presence of a catalyst. The catalyst can be an acid, alkyl ester, or anhydride, such as H2SO4, Me2SO4, or SO3. For example, reaction of 4-methylpyrazole with MeOH in the presence of H2SO4 at 145° gave 1,4-dimethylpyrazole in 94.4% yield.  
 IT 66870-43-7p, 1-Methyl-5-(4-methylphenyl)-3-phenylpyrazole  
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)  
 (product; N-alkylation of pyrazoles with alcs. or esters using acid-type catalysts)  
 RN 66870-43-7 CAPLUS  
 CN 1H-Pyrazole, 1-methyl-5-(4-methylphenyl)-3-phenyl- (9CI) (CA INDEX NAME)

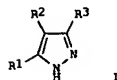


*should be subst.*

L26 ANSWER 30 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1996:504142 CAPLUS  
 DOCUMENT NUMBER: 125:142724  
 TITLE: Preparation of 3,5-diarylpyrazoles from 1,3-diarylpropanones and hydrazine hydrate in the presence of iodine or iodine compounds and sulfuric acid  
 INVENTOR(S): Merkle, Hans Rupert; Fretschner, Erich  
 PATENT ASSIGNEE(S): BASF A.-G., Germany  
 SOURCE: Ger. Offen., 7 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19500838	A1	19960718	DE 1995-19500838	19950113
IN 193044	A1	20040626	IN 1995-MA1718	19951227
CA 2209486	A1	19960718	CA 1996-2209486	19960104
WO 9621650	A1	19960718	WO 1996-EP11	19960104
W: AU, CA, CN, JP, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9644367	A	19960731	AU 1996-44367	19960104
AU 703688	B2	19990401		
EP 802906	A1	19971029	EP 1996-900559	19960104
EP 802906	B1	20051123		
R: AT, BE, CH, DE, ES, FR, GB, IT, LI, NL				
CN 1168136	A	19971217	CN 1996-191420	19960104
CN 1068589	B	20010718		
JP 10511969	T	19981117	JP 1996-521414	19960104
AT 310729	T	20051215	AT 1996-900559	19960104
ES 2255072	T3	20060616	ES 1996-900559	19960104
US 5744614	A	19980428	US 1997-860026	19970703
PRIORITY APPLN. INFO.:				
DE 1995-19500838 A 19950113				
WO 1996-EP11 W 19960104				

OTHER SOURCE(S): CASREACT 125:142724; MARPAT 125:142724  
 GI

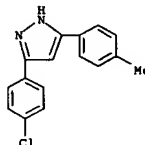


AB 3,5-Diarylpyrazoles [I; R1, R3 = (un)substituted aryl; R2 = H, alkyl, (un)substituted aryl] are prepared in high yield by the reaction of hydrazine hydrate, I or I compds., H2SO4, and a 1,3-diarylpropanone R1CH:C(R2)COR3, or by the reaction of hydrazine hydrate, I or I compds., H2SO4, a carbonyl compound R3COCH2R2, and an aryl aldehyde R1CHO. Thus, a mixture of hydrazine hydrate, 4-methylacetophenone, 4-chlorobenzaldehyde, and NaI was dripped into H2SO4, producing 3-(4-chlorophenyl)-5-(4-methylphenyl)pyrazole, m.p. 228°, in 92% theor. yield.  
 IT 131138-54-OP  
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP

Karen Cheng

L26 ANSWER 30 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

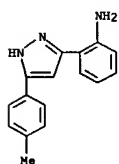
(Preparation)  
 (prepn. of 3,5-diarylpyrazoles from 1,3-diarylpropanones and hydrazine hydrate in the presence of iodine or iodine compds. and sulfuric acid)  
 RN 131138-54-0 CAPLUS  
 CN 1H-Pyrazole, 3-(4-chlorophenyl)-5-(4-methylphenyl)- (9CI) (CA INDEX NAME)



*1025  
claims 1-2  
103  
claim 3*

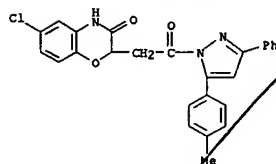
# 10526940species

L26 ANSWER 31 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1996:382875 CAPLUS  
 DOCUMENT NUMBER: 125:75329  
 TITLE: Synthesis and Binding Activity of Some Pyrazolo[1,5-c]quinazolines as Tools To Verify an Optional Binding Site of a Benzodiazepine Receptor Ligand  
 AUTHOR(S): Colotta, Vittoria; Catarzi, Daniela; Varano, Flavia; Filacchioni, Guido; Cecchi, Lucia; Galli, Alessandro; Costagli, Chiara  
 CORPORATE SOURCE: Dipartimento di Scienze Farmaceutiche, Università di Firenze, Florence, 50121, Italy  
 SOURCE: Journal of Medicinal Chemistry (1996), 39(15), 2915-2921  
 CODEN: JMCHAR; ISSN: 0022-2623  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The synthesis and binding activity at the benzodiazepine receptor of some 2-substituted pyrazolo[1,5-c]quinazolines are reported. The structure-activity relationships and in vitro efficacy of the title compds., which are devoid of the proton acceptor atom at position 1, are similar to those of some previously reported tricyclic heteroarom. compds. This suggests that a proton acceptor at position 1 is an optional binding site of a benzodiazepine receptor ligand which only affects potency.  
 IT 178625-21-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and binding activity of pyrazoloquinazolines as tools to verify an optional binding site of a benzodiazepine receptor ligand)  
 RN 178625-21-3 CAPLUS  
 CN Benzenamine, 2-[5-(4-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

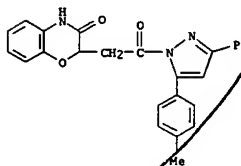


102b  
claim 1-2  
103  
claim 3

L26 ANSWER 32 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



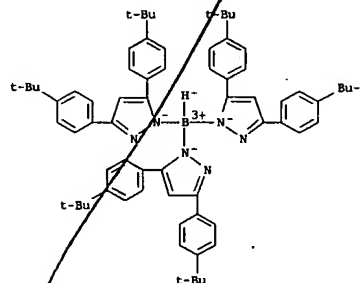
L26 ANSWER 32 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1995:681195 CAPLUS  
 DOCUMENT NUMBER: 123:285925  
 TITLE: Synthesis and biological activities of 1-[(3,4-dihydro-3-oxo-2H-1,4-benzoxazin-2-yl)acetyl]-3,4-disubstituted pyrazoles and 3-methylpyrazoliones  
 AUTHOR(S): Jayaram, V.; Reddy, V. Malli  
 CORPORATE SOURCE: College of Pharmaceutical Sciences, Kakatiya University, Warangal, 506009, India  
 SOURCE: Indian Journal of Pharmaceutical Sciences (1994), 56(4), 132-5  
 CODEN: IJSDIW; ISSN: 0250-474X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 123:285925  
 AB The title compds., i.e., 2-[2-oxo-2-(oxopyrazol-1-yl)ethyl]-2H-benzoxazin-3(4H)-ones were prepared and tested for their antimicrobial activity.  
 IT 169760-48-9P 169760-53-6P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
 (preparation of [oxo(oxopyrazolyl)ethyl]benzoxazinones as antimicrobial agents)  
 RN 169760-48-9 CAPLUS  
 CN 1H-Pyrazole, 1-[(3,4-dihydro-3-oxo-2H-1,4-benzoxazin-2-yl)acetyl]-5-(4-methylphenyl)-3-phenyl- (9CI) (CA INDEX NAME)



RN 169760-53-6 CAPLUS  
 CN 1H-Pyrazole, 1-[(6-chloro-3,4-dihydro-3-oxo-2H-1,4-benzoxazin-2-yl)acetyl]-5-(4-methylphenyl)-3-phenyl- (9CI) (CA INDEX NAME)

L26 ANSWER 33 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1994:93964 CAPLUS  
 DOCUMENT NUMBER: 120:93964  
 TITLE: The synthesis of [HB[3,5-(tert-Buph)2pz]3]- (tert-Buph = p-C6H4-tert-Bu), a new tris(pyrazolyl)hydroborate ligand: the crystal and molecular structure of Tl(n3-HB[3,5-(tert-Buph)2pz]3)  
 AUTHOR(S): Libertini, Emanuela; Yoon, Keum; Parkin, Gerard  
 CORPORATE SOURCE: Dep. Chem., Columbia Univ., NY, 10527, USA  
 SOURCE: Polyhedron (1993), 12(20), 2539-42  
 CODEN: PLYHDE; ISSN: 0277-5387  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The synthesis of a new sterically demanding tris(pyrazolyl)hydroborate ligand, [HB[3,5-(tert-Buph)2pz]3]- (tert-Buph = p-C6H4(OMe3)), is reported. The K derivative is prepared by the direct reaction of KBH4 with 3,5-bis(p-tert-butylphenyl)pyrazole. Metathesis with TlNO3 converts the K derivative to the Tl complex Tl(n3-HB[3,5-(tert-Buph)2pz]3). The crystal and mol. structures of the pyrazole derivative [3,5-(tert-Buph)2pz]2ZnI2 and the Tl derivative Tl(n3-HB[3,5-(tert-Buph)2pz]3) were determined  
 IT 152692-47-2P 152728-23-9P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and crystal structure of)  
 RN 152692-47-2 CAPLUS  
 CN Borate(1-), tris[3,5-bis[4-(1,1-dimethylethyl)phenyl]-1H-pyrazolato-N1]hydro-, thallium(1+), (T-4)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

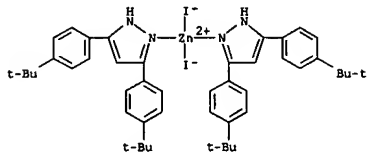
● Tl(I) +

RN 152728-23-9 CAPLUS  
 CN Zinc, bis[3,5-bis[4-(1,1-dimethylethyl)phenyl]-1H-pyrazole-N2]diiodo-, (T-4)- (9CI) (CA INDEX NAME)

Karen Cheng

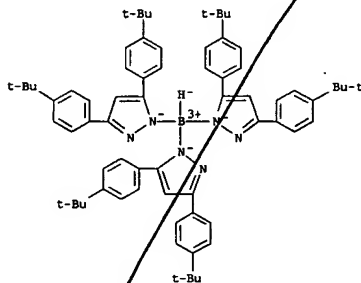
# 10526940species

L26 ANSWER 33 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



IT 152692-46-1P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and metathesis of, with thallium nitrate)  
 RN 152692-46-1 CAPLUS  
 CN Borate(1-), tris[3,5-bis[4-(1,1-dimethylethyl)phenyl]-1H-pyrazolato-N1]hydro-, potassium, (T-4)- (9CI) (CA INDEX NAME)

PAGE 1-A

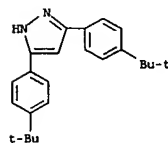


PAGE 2-A

● K<sup>+</sup>

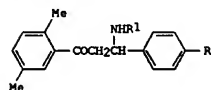
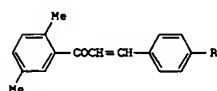
IT 152503-09-8P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

L26 ANSWER 33 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
 (Reactant or reagent)  
 (prepn. and reaction of, with potassium borohydride)  
 RN 152503-09-8 CAPLUS  
 CN 1H-Pyrazole, 3,5-bis[4-(1,1-dimethylethyl)phenyl]- (9CI) (CA INDEX NAME)

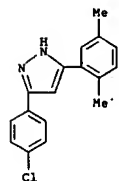


L26 ANSWER 34 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1993:212582 CAPLUS  
 DOCUMENT NUMBER: 118:212582  
 TITLE: Synthesis and some reactions of benzylidene acetophenone derivatives  
 AUTHOR(S): El-Bahaie, S.; Bayoumy, B. E.; El-Mobayed, M.; Abd El-Latif, G.  
 CORPORATE SOURCE: Fac. Sci., Zagazig Univ., Zagazig, Egypt  
 SOURCE: Egyptian Journal of Chemistry (1991), Volume Date 1990, 33(5), 429-38  
 CODEN: EGCJCA3; ISSN: 0367-0422  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

L26 ANSWER 34 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



AB Benzylideneacetophenones I (R = Cl, NO<sub>2</sub>) react are epoxidized to give the corresponding oxiranes. Amination of I with R<sub>1</sub>NH<sub>2</sub> (R<sub>1</sub> = CH<sub>2</sub>Ph, 4-MeOC<sub>6</sub>H<sub>4</sub>) gave aminated derivs. II. I and other derivs. of I underwent various other reactions.  
 IT 146529-43-3P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 146529-43-3 CAPLUS  
 CN 1H-Pyrazole, 3-(4-chlorophenyl)-5-(2,5-dimethylphenyl)- (9CI) (CA INDEX NAME)



Karen Cheng

1026  
 Claim 1-2  
 103  
 claim 3

## 10526940species

L26 ANSWER 35 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1992:633220 CAPLUS

DOCUMENT NUMBER: 117:233220

TITLE: Degenerate and nondegenerate reversible [1,7] O .dblharv. O' alkylotropy of 1-hydroxypyrazole 2-oxides. Variation of channels of associated molecular rearrangements

AUTHOR(S): Olekhnovich, L. P.; Tkachuk, A. V.; Budarina, Z. N.; Ivakhnenko, E. P.; Tseimakh, I. D.; Knyazev, A. P.; Zhdanov, Yu. A.

CORPORATE SOURCE: Rostov. Gos. Univ., Rostov, USSR  
SOURCE: Doklady Akademii Nauk SSSR (1991), 321(3), 530-7 [Chem.]

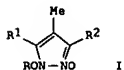
CODEN: DANKAS; ISSN: 0002-3264

DOCUMENT TYPE: Journal

LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 117:233220

GI



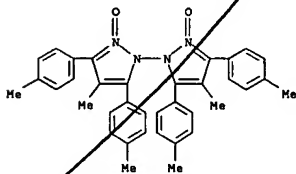
AB Rearrangements in alkoxy-pyrazole oxides I (R = Me, PhCH<sub>2</sub>; R<sub>1</sub>, R<sub>2</sub> = Ph, p-tolyl, Me) occurred by [1,7]-O .dblharv. O' shift of R, [1,5]-N + C and/or [1,3]-N + C shift of RO, and, in the case of R = PhCH<sub>2</sub>, homolytic N-O bond cleavage. Kinetic data were obtained.

IT

RL: PREP (Preparation)  
(formation and dissociation of, kinetics of)

RN 139911-54-9 CAPLUS

CN 1,1'-Bi-1H-pyrazole, 4,4'-dimethyl-3,3',5,5'-tetrakis(4-methylphenyl)-, 2,2'-dioxide (9CI) (CA INDEX NAME)



IT 139911-42-5 139911-44-7

RL: RCT (Reactant); RACT (Reactant or reagent)

L26 ANSWER 36 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:4439 CAPLUS

DOCUMENT NUMBER: 117:171439

TITLE: Preparation of 3-[3(5)-pyrazolyl or isoxazolyl]aniline derivatives and herbicides containing them  
INVENTOR(S): Koyanagi, Hiroshi; Nishisaka, Takashi; Yoshida, Shigeo  
PATENT ASSIGNEE(S): SDS Biotech K. K., Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.

CODEN: JKXXAF

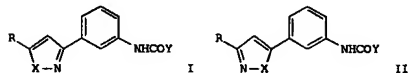
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04124178	A	19920424	JP 1990-241616	19900912
PRIORITY APPL. INFO.:			JP 1990-241616	19900912
OTHER SOURCE(S):				
GI				



AB The title derivs. I (R = lower alkyl, (un)substituted Ph; X = NH, NMe, O; Y = lower alkyl, lower alkenyl, lower alkoxy, lower alkenyloxy, N,N-dialkylamino, N-lower alkyl-N-lower alkoxyamino) or II and herbicides containing I or II are claimed. GlucoMe was added dropwise to 3-tert-butyl-5-(3-aminophenyl)pyrazole (prepared by reduction of the corresponding nitro compound) in pyridine at 0° and the reaction mixture was further stirred at room temperature for 5 h to give 90% I (R = Me, X = NH, Y = OMe) (III). III at 4 kg active ingredient/ha completely controlled barnyard grass, Scirpus juncoides, Monochoria vaginalis, and Ammannia multiflora grown on paddy field without any damage to rice plant.

IT

143704-56-7P 143704-57-9P 143704-58-9P  
143704-59-0P 143704-60-3P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of, as herbicide)

RN 143704-56-7 CAPLUS

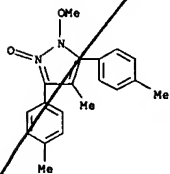
CN Carbanic acid, [3-[5-(2-methylphenyl)-1H-pyrazol-3-yl]phenyl]-, methyl ester (9CI) (CA INDEX NAME)

L26 ANSWER 35 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

(rearrangement of, kinetics and mechanism of)

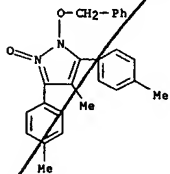
RN 139911-42-5 CAPLUS

CN 1H-Pyrazole, 1-methoxy-4-methyl-3,5-bis(4-methylphenyl)-, 2-oxide (9CI) (CA INDEX NAME)



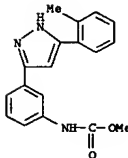
RN 139911-44-7 CAPLUS

CN 1H-Pyrazole, 4-methyl-3,5-bis(4-methylphenyl)-1-(phenylmethoxy)-, 2-oxide (9CI) (CA INDEX NAME)



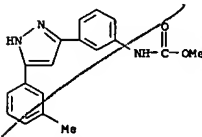
L26 ANSWER 36 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN

(Continued)



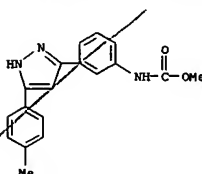
RN 143704-57-8 CAPLUS

CN Carbanic acid, [3-[5-(3-methylphenyl)-1H-pyrazol-3-yl]phenyl]-, methyl ester (9CI) (CA INDEX NAME)



RN 143704-58-9 CAPLUS

CN Carbanic acid, [3-[5-(4-methylphenyl)-1H-pyrazol-3-yl]phenyl]-, methyl ester (9CI) (CA INDEX NAME)



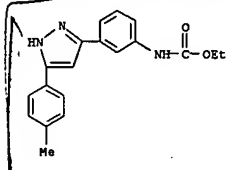
RN 143704-59-0 CAPLUS

CN Carbanic acid, [3-[5-(4-methylphenyl)-1H-pyrazol-3-yl]phenyl]-, ethyl ester (9CI) (CA INDEX NAME)

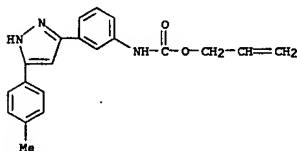
Karen Cheng

## 10526940species

L26 ANSWER 36 OF 56 CAPIUS COPYRIGHT 2007 ACS on STN (Continued)



RN 143704-60-3 CAPIUS  
 CN Carbanic acid, [3-[5-(4-methylphenyl)-1H-pyrazol-3-yl]phenyl]-, 2-propenyl ester (9CI) (CA INDEX NAME)



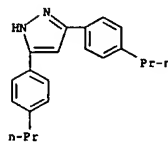
L26 ANSWER 37 OF 56 CAPIUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1992:561422 CAPIUS  
 DOCUMENT NUMBER: 117:161422  
 TITLE: Synthesis and mesomorphic properties of the 3,5-bis-alkoxyphenyl-pyrazoles and -isoxazoles  
 AUTHOR(S): Bartulin, J.; Martinez, R.; Mueller, H. J.; Fan, Z. X.; Haase, W.  
 CORPORATE SOURCE: Fac. Cienc., Univ. Concepcion, Chile  
 SOURCE: Molecular Crystals and Liquid Crystals Science and Technology, Section A: Molecular Crystals and Liquid Crystals (1992), 220, 67-75  
 CODEN: MCLCES; ISSN: 1058-725X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

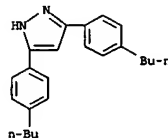
AB The synthesis and measurement of phys. properties using DSC, x-ray and optical methods are described for the 3,5-bis(p-alkoxyphenyl)pyrazole and 3,5-bis(p-alkoxyphenyl)isoxazole series with the C number of the alkyl group from 3 to 8. The pyrazole series with longer alkyl groups (6, 7, and 8) show the smectic A as well as smectic C phases. The corresponding isoxazole compds. show nematic and also smectic A phases. The compds. with shorter alkyl groups (3, 4 and 5) show either nematic or smectic A phases for both series, resp.

IT 143613-60-9P 143613-61-0P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and liquid crystal properties of)

RN 143613-60-9 CAPIUS  
 CN 1H-Pyrazole, 3,5-bis(4-propylphenyl)- (9CI) (CA INDEX NAME)



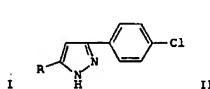
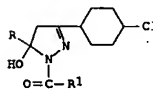
RN 143613-61-0 CAPIUS  
 CN 1H-Pyrazole, 3,5-bis(4-butylphenyl)- (9CI) (CA INDEX NAME)



L26 ANSWER 37 OF 56 CAPIUS COPYRIGHT 2007 ACS on STN (Continued)

L26 ANSWER 38 OF 56 CAPIUS COPYRIGHT 2007 ACS on STN

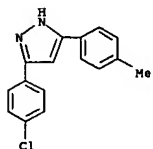
ACCESSION NUMBER: 1991:23863 CAPIUS  
 DOCUMENT NUMBER: 114:23863  
 TITLE: Reactions of aroylhydrazines with chalcone dibromides  
 AUTHOR(S): Holla, B. Shivarama; Udupa, K. Venkatramana  
 CORPORATE SOURCE: Dep. P G Stud. Res. Chem., Mangalore Univ., Mangalagangothri, 574 199, India  
 SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1990), 29B (9), 887-9  
 CODEN: IJCSDB; ISSN: 0376-4699  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 114:23863  
 GI



AB Cyclization of p-ClCGH4CH(Br)CH(Br)C(O)R (R = Ph, p-tolyl, p-ClCGH4) with R1C(O)NHNH2 (R1 = Ph, o-, p-ClCGH4, p-HOCGH4, 2-naphthylomethyl) gave 60-94% 13 pyrazolines I, which underwent acid catalyzed dehydration to give 75-80% pyrazoles II.

IT 131138-54-0P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

RN 131138-54-0 CAPIUS  
 CN 1H-Pyrazole, 3-(4-chlorophenyl)-5-(4-methylphenyl)- (9CI) (CA INDEX NAME)





103 art

L26 ANSWER 42 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

Cc1ccc(cc1)C2=C(C(=[N+]2C)C)C3=CC=C(C)C3Cc1ccc(S(=O)(=O)O)cc1

Q 1

$$\left[ \begin{array}{c} \text{R}^1 \\ \diagup \quad \diagdown \\ \text{R}^5 \quad \text{NR}^2 \\ | \quad | \\ \text{R}^4 \quad \text{R}^3 \end{array} \right] \quad (\text{X}^-)^m \quad \text{I}$$

IT 43222-79-3 58538-73-1  
RL: BIOL (Biological study)  
(plant growth inhibitor, for sunflower)

CH 1

CRN 49867-86-9  
CMF C19 H21 N2

Cc1ccc(cc1)C2=C(C(=[N+]2C)C)C3=CC=C(C=C3)F

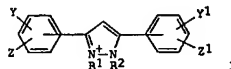
CH 2

CRN 21228-90-0  
CMF C H3 04 S

L26 ANSWER 43 OF 56 CAPLUS COPYRIGHT 2007 ACS on STM

ACCESSION NUMBER: 1980:17174 CAPJUS  
DOCUMENT NUMBER: 92:17174  
TITLE: Herbicidal combinations  
INVENTOR(S): Feeny, Richard W.  
PATENT ASSIGNEE(S): American Cyanamid Co., USA  
SOURCE: U.S., 13 pp  
CODEN: USIOXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 3  
PATENT INFORMATION:

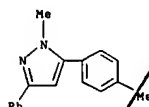
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4170464	A	19791009	US 1977-822504	19770808
US 3867403	A	19750218	US 1972-307670	19721117
PRIORITY APPLN. INFO.:			US 1972-307670	A3 19721117
			US 1974-518070	A2 19741025



AB Mixts. of 1,2-dialkyl-3,5-diphenylpyrazolium salts and chlorophenoxalkanoates or the diphenylpyrazolium chlorophenoxalkanoates I (R1 and R2 = alkyl; R3 = Cl or Me; R4 = H or Me; Y, Y1, Z, Z1 = H, halo, Me, or MeO) are synergistic herbicides. Thus, a composition containing 1,2-dimethyl-3,5-diphenylpyrazolium Me sulfate (43222-48-6) (1.12 kg/ha) and 2,4-d-dimethylamine salt [2008-39-1] (0.56 kg/ha) almost totally controlled the weeds in the winter wheat and shepherd's purse, with min. phytotoxicity to winter wheat, whereas the pyrazolium compound by itself showed little herbicidal activity.

IT 66870-43-7P 72218-38-3P 72218-42-9P  
72218-43-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)

RN 66870-43-7 CAPLUS  
 CN 1H-Pyrazole, 1-methyl-5-(4-methylphenyl)-3-phenyl- (9CI) (CA INDEX NAME)



RN 72218-38-3 CAPLUS  
CN 1H-Pyrazole, 5-(2,6-dimethylphenyl)-1-methyl-3-phenyl- (9CI) (CA INDEX

Karen Cheng

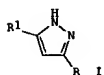
not  
only.

## 10526940species

L26 ANSWER 46 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1976:433005 CAPLUS  
 DOCUMENT NUMBER: 85:33005  
 TITLE: Pyrazole plant growth regulants  
 INVENTOR(S): Johnson, Alexander Lawrence; Sweetser, Philip B.  
 PATENT ASSIGNEE(S): du Pont de Nemours, E. I., and Co., USA  
 SOURCE: U.S., 15 pp  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3948937	A	19760406	US 1973-397720	19730917
IL 39092	A	19760229	IL 1972-39092	19720327
IT 955155	B	19730929	IT 1972-22831	19720407
AU 7241026	A	19731018	AU 1972-41026	19720412
ZA 7202576	A	19730131	ZA 1972-2576	19720417
ES 401879	A1	19760201	ES 1972-401879	19720418
CA 982588	A1	19760127	CA 1972-140051	19720419
BR 7202417	DO	19730503	BR 1972-2417	19720420
NL 7205441	A	19721024	NL 1972-5441	19720421
FR 2136595	A5	19721222	FR 1972-14198	19720421
JP 58011401	B	19830302	JP 1972-39729	19720421
US 4055409	A	19771025	US 1975-627462	19751030
PRIORITY APPLN. INFO.:			US 1971-136576	A2 19710422
			US 1972-230508	A2 19720229
			US 1973-397720	A3 19730917

GI

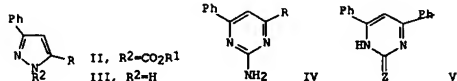


AB Pyrazoles (I, R = 2-HO<sub>2</sub>CC<sub>6</sub>H<sub>4</sub>, substituted 2-carboxyphenyl; R1 = Ph, substituted phenyl) (35 compds.) were prepared. Thus, 100 g di-Na salt of 2-benzoylacetylbenzoic acid in MeOH-HCl was cyclized with 11 g NH<sub>2</sub>NH<sub>2</sub> to give 59 g of I (R = 2-HO<sub>2</sub>CC<sub>6</sub>H<sub>4</sub>, R1 = Ph). I at low rates, 0.001 - 4 lb/acre, are plant growth regulators and at higher rates, 0.5-10 lb/acre, exhibit herbicidal activity.

IT 39784-92-4P 39784-96-8P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

RN 39784-92-4 CAPLUS  
 CN Benzoic acid, 2-[5-(4-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

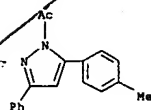
L26 ANSWER 47 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1976:432950 CAPLUS  
 DOCUMENT NUMBER: 85:32950  
 TITLE: Acetylinic ketones. Part II. Reaction of acetylinic ketones with nucleophilic nitrogen compounds  
 AUTHOR(S): Baddar, F. G.; Al-Hajjaj, F. H.; El-Rayyes, N. R.  
 CORPORATE SOURCE: Dep. Chem., Kuwait Univ., Kuwait, Kuwait  
 SOURCE: Journal of Heterocyclic Chemistry (1976), 13(2), 257-68  
 CODEN: JHCTAD; ISSN: 0022-152X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 85:32950



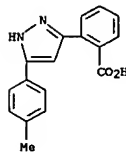
AB PhC.tplbond.COOR [I, R = Ph, C<sub>6</sub>H<sub>4</sub>Me-p, C<sub>6</sub>H<sub>4</sub>Cl-m, p, C<sub>6</sub>H<sub>4</sub>OMe-p, 3,4-(methylenedioxy)phenyl] reacted with H<sub>2</sub>NNHCO<sub>2</sub>R1 (R1 = Ph, Et) to give ROOCH:CPHNNHCO<sub>2</sub>R1, which were cyclized with Ac<sub>2</sub>O to give the pyrazolecarboxylates II, which on hydrolysis-decarboxylation with MeOH-NaOH gave the aromatic pyrazoles III; I also reacted with NH<sub>2</sub>C(=NH)NH<sub>2</sub> to give the pyrimidines IV; similarly, the pyrimidines V (Z = S, O) were prepared from heating PhC.tplbond.COOPh with H<sub>2</sub>NZC(=Z)NH<sub>2</sub>.

IT 59807-09-9P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

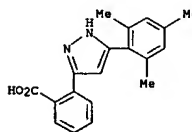
RN 59807-09-9 CAPLUS  
 CN 1H-Pyrazole, 1-acetyl-5-(4-methylphenyl)-3-phenyl- (9CI) (CA INDEX NAME)



L26 ANSWER 46 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 39784-96-8 CAPLUS  
 CN Benzoic acid, 2-[5-(2,4,6-trimethylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



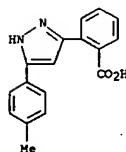
102b = 192  
 103 = 3

L26 ANSWER 48 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1976:131323 CAPLUS  
 DOCUMENT NUMBER: 84:131323  
 TITLE: Effect of substituted pyrazoles and related compounds on geotropism in cress seedlings  
 AUTHOR(S): Geissler, Att E.; Huppertz, John L.; Katekar, Gerard F.  
 CORPORATE SOURCE: Div. Plant Ind., CSIRO, Canberra, Australia  
 SOURCE: Pesticide Science (1975), 6(5), 441-50  
 CODEN: PSSCBG; ISSN: 0031-613X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI For diagram(s), see printed CA Issue.

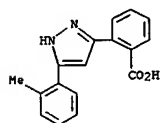
AB 2-Phenyl-8H-pyrazolo[6,1-a]isoindol-8-one (I) [37564-20-8], 5-(2-carboxyphenyl)-3-phenylpyrazole [39784-88-8], and derivs. of both these compds. were highly active against root geotropism in cress seedling, destruction of geotropism occurring at 10<sup>-7</sup>-10<sup>-9</sup>M. Substitution with functional groups and increased mol. size caused only minor variations in activity.

IT 39784-92-4P 58726-52-6P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and geotropic activity of)

RN 39784-92-4 CAPLUS  
 CN Benzoic acid, 2-[5-(4-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



RN 58726-52-6 CAPLUS  
 CN Benzoic acid, 2-[5-(2-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



## 10526940species

L26 ANSWER 49 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1976:116915 CAPLUS  
DOCUMENT NUMBER: 84:116915  
TITLE: Pyrazolium fungicides  
INVENTOR(S): Walworth, Bryant L.  
PATENT ASSIGNEE(S): American Cyanamid Co., USA  
SOURCE: U.S., 10 pp.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 7  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3930011	A	19751230	US 1975-546654	19750203
ZA 7507951	A	19761229	ZA 1975-7951	19751222
IL 48708	A	19780731	IL 1975-48708	19751223
AU 7587903	A	19770630	AU 1975-87903	19751224
AU 500653	B2	19790531		
GB 1534866	A	19781206	GB 1975-53214	19751230
CA 1058517	A1	19790717	CA 1976-243287	19760109
NL 7600700	A	19760805	NL 1976-700	19760123
DK 7600296	A	19760804	DK 1976-296	19760126
DK 139833	C	19791001		
DK 139833	B	19790430		
FI 7600174	A	19760804	FI 1976-174	19760126
FI 59194	B	19810331		
FI 59194	C	19810710		
DE 2602964	A1	19760805	DE 1976-2602964	19760127
CS 199651	B2	19800731	CS 1976-580	19760129
DE 838171	A4	19760802	DE 1976-164007	19760202
SE 7601095	A	19760803	SE 1976-1095	19760202
SE 420888	B	19811109		
SE 420888	C	19820218		
NO 7600343	A	19760804	NO 1976-343	19760202
NO 145039	B	19810921		
NO 145039	C	19820104		
BR 7600646	A	19760831	BR 1976-646	19760202
CH 594354	A5	19780113	CH 1976-1243	19760202
AT 347178	B	19781211	AT 1976-697	19760202
SU 644359	A3	19790125	SU 1976-2319208	19760202
FR 2298949	A2	19760827	FR 1976-2975	19760203
FR 2298949	B2	19790330		
JP 51104031	A	19760914	JP 1976-10777	19760203
DD 124703	A6	19770309	DD 1976-191070	19760203
			US 1971-209448	A 19711217
			US 1972-271424	A 19720713
			GB 1972-55680	A 19721201
			US 1975-546654	A 19750203

GI

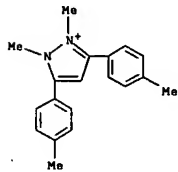
L26 ANSWER 49 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 43222-78-2 CAPLUS  
CN 1H-Pyrazolium, 1,2-dimethyl-3,5-bis(4-methylphenyl)-, methyl sulfate (9CI)  
(CA INDEX NAME)

CH 1

CRN 49867-86-9  
CHF C19 H21 N2



CH 2

CRN 21228-90-0  
CHF C H3 O4 S

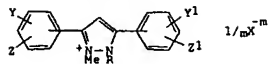
Me-O-SO3-

RN 43222-79-3 CAPLUS  
CN 1H-Pyrazolium, 1,2-dimethyl-3,5-bis(4-methylphenyl)-, salt with 4-methylbenzenesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CH 1

CRN 49867-86-9  
CHF C19 H21 N2

L26 ANSWER 49 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



AB Dialkylidiphenylpyrazolium salts I (R=alkyl, allyl, propynyl, ethylcarboxymethyl, Ph, or PhCH2; Y, Y', Z, and Z'=H, halogen, Cl-4 alkyl or alkoxy; X=mono- or divalent anion; m = 1 or 2) were effective as fungicides. For example, 1,2-dimethyl-3,5-diphenylpyrazolium methyl sulfate (43222-48-6) was effective for control of Phytophthora infestans on tomato, Piricularia oryzae on rice, and Venturia inaequalis on apple. The synthesis of I is described.

IT 43222-60-2P 43222-78-2P 43222-79-3P  
58538-18-4P 58538-19-5P 58538-21-9P  
58538-22-0P 58538-34-4P 58538-37-7P  
58538-38-8P 58538-47-9P 58538-59-3P  
58538-67-3P 58538-68-4P 58538-73-1P  
58538-74-2P

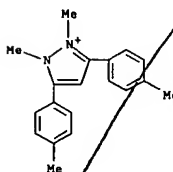
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation and fungicidal activity of)

RN 43222-60-2 CAPLUS

CN 1H-Pyrazolium, 1,2-dimethyl-3,5-bis(4-methylphenyl)-, perchlorate (9CI)  
(CA INDEX NAME)

CH 1

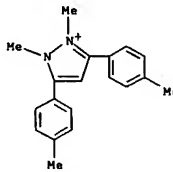
CRN 49867-86-9  
CHF C19 H21 N2



CH 2

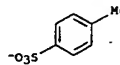
CRN 14797-73-0  
CHF C1 O4

L26 ANSWER 49 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CH 2

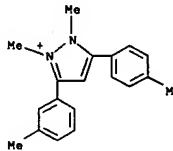
CRN 16722-51-3  
CHF C7 H7 O3 S



RN 58538-18-4 CAPLUS  
CN 1H-Pyrazolium, 1,2-dimethyl-3-(3-methylphenyl)-5-(4-methylphenyl)-, methyl sulfate (9CI) (CA INDEX NAME)

CH 1

CRN 58538-17-3  
CHF C19 H21 N2



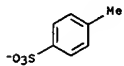
CH 2

CRN 21228-90-0  
CHF C H3 O4 S

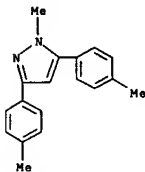
Karen Cheng

## 10526940species

L26 ANSWER 52 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



IT 43222-89-5  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (quaternization of)  
 RN 43222-89-5 CAPLUS  
 CN 1H-Pyrazole, 1-methyl-3,5-bis(4-methylphenyl)- (9CI) (CA INDEX NAME)

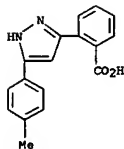


L26 ANSWER 53 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1973:58410 CAPLUS  
 DOCUMENT NUMBER: 78:58410  
 TITLE: Plant growth regulating 3,5-diphenylpyrazoles  
 INVENTOR(S): Johnson, Alexander Lawrence; Sweetser, Philip Bliss  
 du Pont de Nemours, E. I., and Co.  
 PATENT ASSIGNEE(S): Ger. Offen., 70 pp.  
 SOURCE: CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

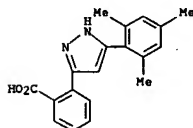
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2219702	A	19721116	DE 1972-2219702	19720421
IL 39092	A	19760229	IL 1972-39092	19720327
IT 955155	B	19730929	IT 1972-22831	19720407
AU 7241026	A	19731018	AU 1972-41026	19720412
ZA 7202576	A	19730131	ZA 1972-2576	19720417
ES 401879	A1	19760201	ES 1972-401879	19720418
CA 982588	A1	19760127	CA 1972-140051	19720419
BR 7202417	D0	19730503	BR 1972-2417	19720420
NL 7205441	A	19721024	NL 1972-5441	19720421
FR 2136595	A5	19721222	FR 1972-14198	19720421
JP 58011401	B	19830302	JP 1972-39729	19720421
PRIORITY APPLN. INFO.:				
US 1971-136576			US 1971-136576	A 19710422
US 1972-230508			US 1972-230508	A 19720229

GI For diagram(s), see printed CA Issue.  
 AB About 30 title compds. (e.g. I, Rn = 4-F, 3-MeO, 4-Me, 3-Br, 2,4,6-Me3, 4-Cl, or 2-MeO; R1 = H or Et; R2 = H, Me, or Ac; R3 = OH, OMe, OEt, OPr, OBu, OCH2CH2OH, CO2H, CONH2, or CONHMe; R4 = H or Me) were prepared either from phthalic anhydride (or its 4-methyl derivative) and MeCOCHGHS-nRn via 2,4-NaO2CR4CGH3COCHNaOCOGHS-nRn and reaction with R2NHNH2 or (in the case of R1 = R2 = R4 = H) by cleavage of II with R3H and optionally Na. I were used against weeds in culture plant fields, e.g. sugar cane, soybean, peanut, or citrus, and for growth regulation of cotton, soybeans, and peanuts.  
 IT 39784-92-4P 39784-96-8P 39785-13-2P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 39784-92-4 CAPLUS  
 CN Benzoic acid, 2-[5-(4-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

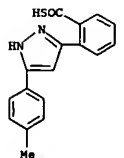
L26 ANSWER 53 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 39784-96-8 CAPLUS  
 CN Benzoic acid, 2-[5-(2,4,6-trimethylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



RN 39785-13-2 CAPLUS  
 CN Benzenecarbothioic acid, 2-[5-(4-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



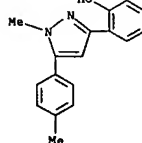
L26 ANSWER 54 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1972:564690 CAPLUS  
 DOCUMENT NUMBER: 77:164690  
 TITLE: Pharmacologically active 5-(o-hydroxyphenyl)pyrazoles  
 INVENTOR(S): Ferlux  
 PATENT ASSIGNEE(S): Fr. Demande, 22 pp.  
 SOURCE: CODEN: FRXXBL  
 DOCUMENT TYPE: Patent  
 LANGUAGE: French  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2104932	A1	19720428	FR 1970-32535	19700908
FR 2104932	A5	19720428		
FR 2104932	B1	19740830		

PRIORITY APPLN. INFO.:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 1970-32535			FR 1970-32535	A 19700908

GI For diagram(s), see printed CA Issue.  
 AB 5-(o-Hydroxyphenyl)pyrazoles I (R = 2-FCGH4, 4-FCGH4, 3,4-Cl2C6-H3, 3,4-(MeO)2C6H3, 4-MeC6H4, 4-(O2N)C6H4, 3-ClC6H4, Ph, 2-furyl; R1 = H, Me, Ph, p-(O2N)C6H4, PhCH2CH2) were prepared. Thus treatment of o-HOC6H4COMe with o-FCGH4COCl gave 2-(o-FCGH4CO2)CGH4COMe, which on treatment with K in pyridine gave the K salt of o-HOC6H4COCH2COCGH4F-o. The latter was cyclized with MeNHNEH2 to I (R = o-FCGH4, R1 = Me). I showed antiinflammatory, analgesic, sedative, diuretic, and hypocholesteremic activity in a variety of tests.  
 IT 38371-76-5P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 38371-76-5 CAPLUS  
 CN Phenol, 2-[1-methyl-5-(4-methylphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



102b = claim 1-3  
 claim 9?

## 10526940species

L26 ANSWER 55 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1964:3172 CAPLUS

DOCUMENT NUMBER: 60:3172

ORIGINAL REFERENCE NO.: 60:527b-c

TITLE: Extrusion of sulfur. VI. Novel ring-contractions giving pyridazines and pyrazoles  
AUTHOR(S): London, J. D.; Young, L. B.  
CORPORATE SOURCE: Univ. Glasgow, UK  
SOURCE: Journal of the Chemical Society (1963), (Nov.), 5496-5502  
CODEN: JCSOA9; ISSN: 0368-1769

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 60:3172

GI For diagram(s), see printed CA issue.  
AB cf. CA 57, 12434f. 2,7-Dihydro-3,6-diphenyl-1,4,5-thiadiazepine (I) yields 3,6-diphenylpyridazine (II) by halogenation-dehalogenation or by thermal decomposition. When heated in acetic acid its S,S-dioxide also yields the pyridazine, whereas its S-monoxide affords 3,5-diphenylpyrazole (III) and hence, in presence of H<sub>2</sub>O<sub>2</sub>, 2,5-diphenyl-1,3,4-oxadiazole (IV) and 1,2-dibenzoylhydrazine. The S,S-dioxide is isomerized by NaOEt-EtOH to a sulfinic acid which loses SO<sub>2</sub> when melted and yields 3-methyl-4,5-diphenylpyrazole (V).

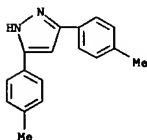
IT 93330-77-9P, Pyrazole, 3,5-di-p-tolyl-

RL: PREP (Preparation)

(preparation of)

RN 93330-77-9 CAPLUS

CN 1H-Pyrazole, 3,5-bis(4-methylphenyl)- (9CI) (CA INDEX NAME)

1024 = 1-2  
103 = 3

L26 ANSWER 56 OF 56 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1939:11351 CAPLUS

DOCUMENT NUMBER: 33:11351

ORIGINAL REFERENCE NO.: 33:1727d-g

TITLE: Reactions of phenylpropiol-4-iodoanilide and similar thioamides  
AUTHOR(S): Worrall, David E.; Lerner, Morris; Washnock, John, Jr.  
SOURCE: Journal of the American Chemical Society (1939), 61, 105-6  
CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB The thioamides were prepared from PhC.tolbond.CNA and the appropriate isothiocyanate in Et<sub>2</sub>O in 60-80% yields; all but the 4-Ph derivative (bright yellow) were pale yellow; the substances were polymerized by heating Et<sub>2</sub>O solns. containing a little NaOH; these are brown or greenish brown and melt with decomposition. Aniline-substituted phenylpropiolthioanilides: 4-I, m. 140-1° (dimer, m. above 173°); 4-Br, m. 111-12° (dimer, m. 199-200°); 3-Br, m. 160-1° (dimer, indefinite m. p.); 4-Ph, m. 128-9° (dimer, m. 230-2°); α-naphthyl, m. 184-5°. NH<sub>2</sub>OH gives 5-phenylisoxazoles in 20-30% yields; 3-(4-iodoanilino), m. 148-9°; 4-Br derivative, m. 172-3°; 4-Cl derivative, m. 151-2°; 4-NH<sub>2</sub> derivative, m. 243-4°; 3-(2-bromo-p-toluidino)-4-bromo, m. 130-1°; 3-(2,6-dichloro-p-toluidino)-4-chloro, m. 229-30°; 3-(4-phenylanilino), m. 176-7°. 5-Phenylpyrazoles: 3-(4-iodoanilino), m. 175-6°; 3-(2-bromo-4-iodoanilino)-4-bromo, m. 201-2°; 3-(4-iodoanilino)-4-chloro, m. 206-7°; 3-(3-bromoanilino), m. 205-6°; 3-(3-bromoanilino)-4-bromo, m. 178-9°; 3-(p-toluidino), m. 157-8°; 3-(2-bromo-p-toluidino)-4-bromo, m. 181-2°; 3-(2,6-dinitro-p-toluidino)-4-nitro, m. 245-7°; 3-(4-phenylanilino), m. 219-20°.

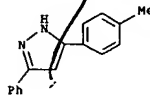
IT 854699-53-9P, Pyrazole, 3-phenyl-5-p-toluidino-

RL: PREP (Preparation)

(preparation of)

RN 854699-53-9 CAPLUS

CN Pyrazole, 3-phenyl-5-p-toluidino- (4CI) (CA INDEX NAME)



10526940claim4

Search Claim4

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT  
MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),  
AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

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NEWS LOGIN Welcome Banner and News Items  
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FILE 'HOME' ENTERED AT 17:14:23 ON 01 MAR 2007

=> fil reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

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STRUCTURE FILE UPDATES: 28 FEB 2007 HIGHEST RN 923894-67-1

DICTIONARY FILE UPDATES: 28 FEB 2007 HIGHEST RN 923894-67-1

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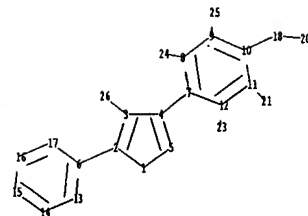
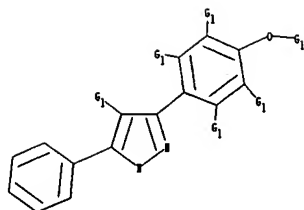
REGISTRY includes numerically searchable data for experimental and  
predicted properties as well as tags indicating availability of  
experimental property data in the original document. For information  
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<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10526940claim4.str

Karen Cheng



chain nodes :  
 18 20 21 23 24 25 26  
 ring nodes :  
 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17  
 chain bonds :  
 2-6 3-26 4-7 8-24 9-25 10-18 11-21 12-23 18-20  
 ring bonds :  
 1-2 1-5 2-3 3-4 4-5 6-13 6-17 7-8 7-12 8-9 9-10 10-11 11-12 13-14  
 14-15 15-16 16-17  
 exact/norm bonds :  
 1-2 1-5 3-26 4-5 8-24 9-25 10-18 11-21 12-23 18-20  
 exact bonds :  
 2-3 2-6 3-4 4-7  
 normalized bonds :  
 6-13 6-17 7-8 7-12 8-9 9-10 10-11 11-12 13-14 14-15 15-16 16-17  
 isolated ring systems :  
 containing 1 : 6 : 7 :

G1:H,CH3

Match level :  
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 20:CLASS  
 21:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS

L1 STRUCTURE UPLOADED

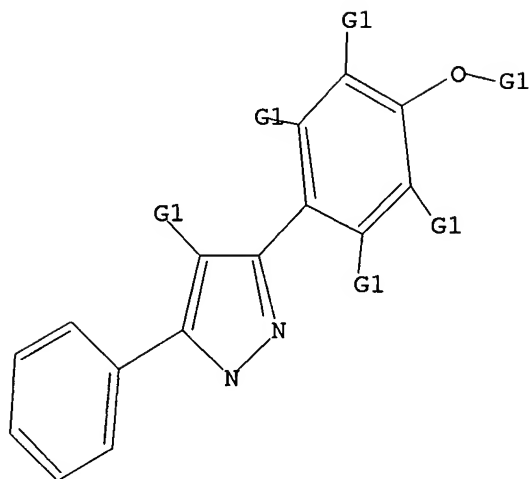
Karen Cheng

10526940claim4

=> d

L1 HAS NO ANSWERS

L1 STR



G1 H, Me

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

FULL SEARCH INITIATED 17:14:48 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 106151 TO ITERATE

100.0% PROCESSED 106151 ITERATIONS

854 ANSWERS

SEARCH TIME: 00.00.01

L2 854 SEA SSS FUL L1

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

172.10

172.31

FILE 'CAPLUS' ENTERED AT 17:14:57 ON 01 MAR 2007

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FILE COVERS 1907 - 1 Mar 2007 VOL 146 ISS 10

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10526940claim4

FILE LAST UPDATED: 28 Feb 2007 (20070228/ED)

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=> s 12

L3            155 L2

=> d ibib abs hitstr 120-155

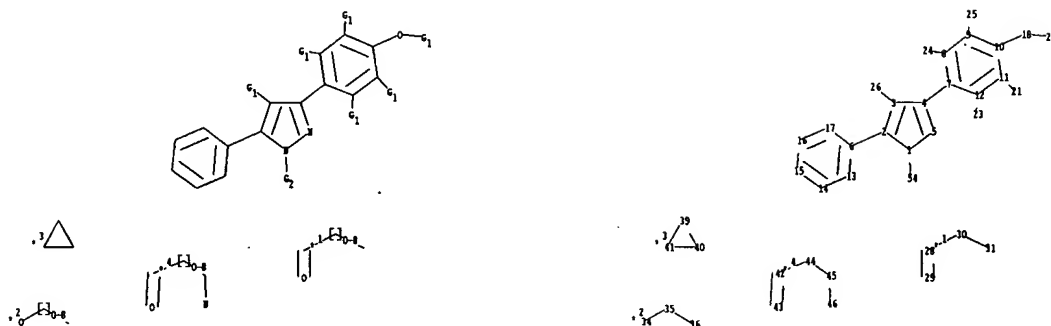
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10526940claim4

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10526940cla4.str



chain nodes :

18 20 21 23 24 25 26 28 29 30 31 34 35 36 42 43 44 45 46 54

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 39 40 41

chain bonds :

1-54 2-6 3-26 4-7 8-24 9-25 10-18 11-21 12-23 18-20 28-30 28-29 30-31  
34-35 35-36 42-43 42-44 44-45 45-46

ring bonds :

1-2 1-5 2-3 3-4 4-5 6-13 6-17 7-8 7-12 8-9 9-10 10-11 11-12 13-14  
14-15 15-16 16-17 39-40 39-41 40-41

exact/norm bonds :

1-2 1-5 1-54 3-26 4-5 8-24 9-25 10-18 11-21 12-23 18-20 28-29 34-35  
42-43 45-46

exact bonds :

2-3 2-6 3-4 4-7 28-30 30-31 35-36 39-40 39-41 40-41 42-44 44-45

normalized bonds :

6-13 6-17 7-8 7-12 8-9 9-10 10-11 11-12 13-14 14-15 15-16 16-17

isolated ring systems :

containing 1 : 6 : 7 : 39 :

G1:H,CH3

G2:H,Ak, [\*1], [\*2], [\*3], [\*4]

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10526940claim4

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 20:CLASS  
21:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 28:CLASS 29:CLASS 30:CLASS  
31:CLASS 34:CLASS 35:CLASS 36:CLASS 39:Atom 40:Atom 41:Atom 42:CLASS  
43:CLASS 44:CLASS 45:CLASS 46:CLASS 54:CLASS

L6 STRUCTURE UPLOADED

=> d

L6 HAS NO ANSWERS

L6 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=> d his

(FILE 'HOME' ENTERED AT 17:14:23 ON 01 MAR 2007)

FILE 'REGISTRY' ENTERED AT 17:14:32 ON 01 MAR 2007

L1 STRUCTURE UPLOADED

L2 854 S L1 FULL

FILE 'CAPLUS' ENTERED AT 17:14:57 ON 01 MAR 2007

L3 155 S L2

FILE 'REGISTRY' ENTERED AT 17:16:13 ON 01 MAR 2007

L4 STRUCTURE UPLOADED

L5 671 S L4 FULL SUB=L2

FILE 'STNGUIDE' ENTERED AT 17:16:48 ON 01 MAR 2007

FILE 'REGISTRY' ENTERED AT 17:20:20 ON 01 MAR 2007

L6 STRUCTURE UPLOADED

=> s l6 full sub=l2

FULL SUBSET SEARCH INITIATED 17:20:48 FILE 'REGISTRY'

FULL SUBSET SCREEN SEARCH COMPLETED - 854 TO ITERATE

100.0% PROCESSED 854 ITERATIONS

165 ANSWERS

SEARCH TIME: 00.00.01

L7 165 SEA SUB=L2 SSS FUL L6

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

41.10

445.53

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

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10526940claim4

	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-28.08

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=> s 17

L8 73 L7

=> d ibib abs hitstr 50-73

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=> fil reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

127.42

572.95

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-18.72

-46.80

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STRUCTURE FILE UPDATES: 28 FEB 2007 HIGHEST RN 923894-67-1

DICTIONARY FILE UPDATES: 28 FEB 2007 HIGHEST RN 923894-67-1

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TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

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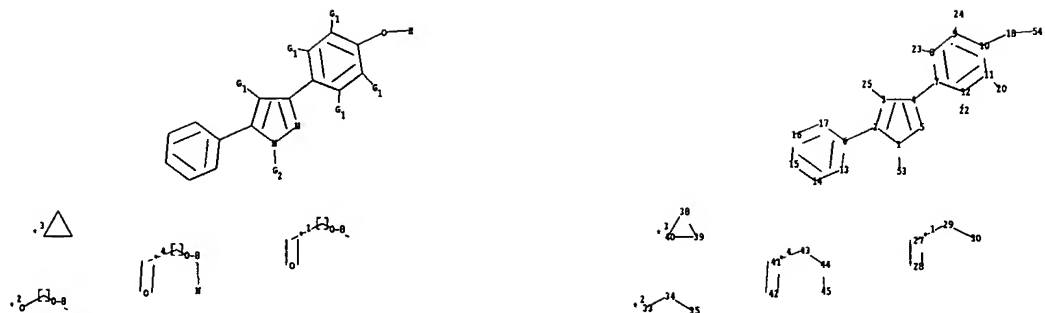
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

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chain nodes :

18 20 22 23 24 25 27 28 29 30 33 34 35 41 42 43 44 45 53 54

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 38 39 40

chain bonds :

1-53 2-6 3-25 4-7 8-23 9-24 10-18 11-20 12-22 18-54 27-29 27-28 29-30  
33-34 34-35 41-42 41-43 43-44 44-45

ring bonds :

1-2 1-5 2-3 3-4 4-5 6-13 6-17 7-8 7-12 8-9 9-10 10-11 11-12 13-14  
14-15 15-16 16-17 38-39 38-40 39-40

exact/norm bonds :

1-2 1-5 1-53 3-25 4-5 8-23 9-24 10-18 11-20 12-22 27-28 33-34 41-42  
44-45

exact bonds :

2-3 2-6 3-4 4-7 18-54 27-29 29-30 34-35 38-39 38-40 39-40 41-43 43-44

normalized bonds :

6-13 6-17 7-8 7-12 8-9 9-10 10-11 11-12 13-14 14-15 15-16 16-17

isolated ring systems :

containing 1 : 6 : 7 : 38 :

G1:H,CH3

G2:H,Ak,[\*1],[\*2],[\*3],[\*4]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 20:CLASS  
22:CLASS 23:CLASS 24:CLASS 25:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS  
33:CLASS 34:CLASS 35:CLASS 38:Atom 39:Atom 40:Atom 41:CLASS 42:CLASS  
43:CLASS 44:CLASS 45:CLASS 53:CLASS 54:CLASS

Karen Cheng

10526940claim4

L9           STRUCTURE UPLOADED

=> d

L9 HAS NO ANSWERS

L9           STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -   AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=> d his

(FILE 'HOME' ENTERED AT 17:14:23 ON 01 MAR 2007)

FILE 'REGISTRY' ENTERED AT 17:14:32 ON 01 MAR 2007

L1           STRUCTURE UPLOADED

L2           854 S L1 FULL

FILE 'CAPLUS' ENTERED AT 17:14:57 ON 01 MAR 2007

L3           155 S L2

FILE 'REGISTRY' ENTERED AT 17:16:13 ON 01 MAR 2007

L4           STRUCTURE UPLOADED

L5           671 S L4 FULL   SUB=L2

FILE 'STNGUIDE' ENTERED AT 17:16:48 ON 01 MAR 2007

FILE 'REGISTRY' ENTERED AT 17:20:20 ON 01 MAR 2007

L6           STRUCTURE UPLOADED

L7           165 S L6 FULL   SUB=L2

FILE 'CAPLUS' ENTERED AT 17:20:51 ON 01 MAR 2007

L8           73 S L7

FILE 'REGISTRY' ENTERED AT 17:21:58 ON 01 MAR 2007

L9           STRUCTURE UPLOADED

=> s l9 full sub=l7

FULL SUBSET SEARCH INITIATED 17:22:31 FILE 'REGISTRY'

FULL SUBSET SCREEN SEARCH COMPLETED -       165 TO ITERATE

100.0% PROCESSED       165 ITERATIONS

100 ANSWERS

SEARCH TIME: 00.00.01

L10           100 SEA SUB=L7 SSS FUL L9

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

41.10

614.05

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10526940claim4

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

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=> s l10

L11 13 L10

=> d ibib abs hitstr tot

Karen Cheng



## 10526940claim4

L11 ANSWER 1 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:1095978 CAPLUS

DOCUMENT NUMBER: 145:438611

TITLE: Preparation of 3,5-diphenylpyrazoles as antitumor agents

INVENTOR(S): Kuroiwa, Shunsuke; Maruyama, Sakiko; Suzuki, Yoshikazu; Yamazaki, Hiroko

PATENT ASSIGNEE(S): Nippon Kayaku Kabushiki Kaisha, Japan

SOURCE: PCT Int. Appl., 45pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

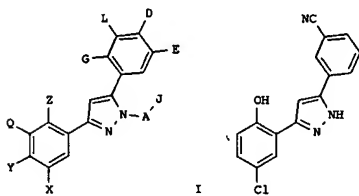
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006:109680	A1	2006:1019	WO 2006-JP307346	2006:0406
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, T, TH, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				

PRIORITY APPLN. INFO.: JP 2005-110717 A 2005:0407

OTHER SOURCE(S): MARPAT 145:438611

GI



AB Title compds. I [wherein A = H, carbonyl or sulfonyl; J = (un)substituted alkyl or amino; G, Z = H, OH, alkoxy, etc.; D, E, L, Q, X, Y = H,

L11 ANSWER 1 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

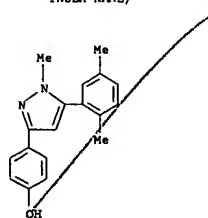
(un)substituted aminocarbonyl, alkoxycarbonyl, etc., D and L, and Q and Y may link together to form a N/S-heterocyclyl ring, with limitations] and pharmaceutically acceptable salts thereof were prepd. as anticancer agents. For instance, treatment of 5'-chloro-2'-hydroxyacetophenone with 3-cyanobenzoyl chloride followed by cyclization with hydrazine hydrate gave diphenylpyrazole II. This product showed cell growth inhibition with IC50 of 0.23 µg/mL against MCF-7 cells and 0.066 µg/mL against MDA-MB-453 cells, resp. Therefore, the invented compds. and their pharmaceutical compns. are useful for the treatment of various cancer, such as breast cancer and lung cancer.

IT RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(reference; preparation of diphenylpyrazoles as antitumor agents)

RN 362006-35-7 CAPLUS

CN Phenol, 4-[5-(2,5-dimethylphenyl)-1-methyl-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

21

THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 2 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:1089202 CAPLUS

DOCUMENT NUMBER: 145:439502

TITLE: Epoxy resin compositions, their epoxides having low melting point, and prepregs thereof

INVENTOR(S): Inoue, Kazuya; Hibino, Hiroaki

PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 22pp.

CODEN: JKKKAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

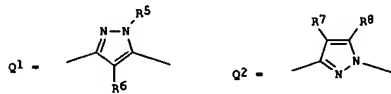
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2006:282531	A	2006:1019	JP 2005-101698	2005:0331
JP 2005-101698				

PRIORITY APPLN. INFO.:

GI



AB The epoxides are G2-p-C6H2R1R2Y-p-C6H2R3R4ZG [G = glycidyl; R1-R4 = H, halo, C1-8 alkyl(oxy), CN, NO2; Y = Q1, Q2 (R5 = H, C1-8 alkyl; R6-R8 = H, C1-8 alkyl, halo, CN, NO2; Z = single bond, O, C1-8 alkylene)]. Thus, 5 g 4-methoxyacetophenone was reacted with 5.5 g Me 4-methoxybenzoate to give 1,3-bis(4-methoxyphenyl)propane-1,3-dione in 83% yield, which was reacted with methylhydrazine, hydrolyzed, and reacted with epichlorohydrin in the presence of tetrabutylammonium bromide to give 3,5-bis(4-(oxiranymethoxy)phenyl)-1-methylpyrazole (I; m.p. 127°) in 91% yield. Then, I was reacted with diaminodiphenylmethane, poured in a mold, and kept at 145-155° and then at 180° to give a cured resin.

IT 912804-13-8P

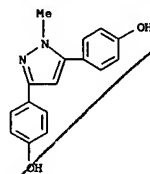
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(pyrazolyl group-containing epoxy compds. and their compns. for forming prepregs)

RN 912804-13-8 CAPLUS

CN Phenol, 4,4'-(1-methyl-1H-pyrazole-3,5-diyl)bis- (9CI) (CA INDEX NAME)

L11 ANSWER 2 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



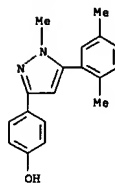
## 10526940claim4

L11 ANSWER 3 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2004:211991 CAPLUS  
 DOCUMENT NUMBER: 140:264528  
 TITLE: NR3B1 nuclear receptor-binding 3-substituted pyrazole derivatives, and therapeutic uses  
 INVENTOR(S): Deuschle, Ulrich; Heck, Stefanie; Kober, Ingo; Bauer, Ulrike; Balogh, Imola  
 PATENT ASSIGNEE(S): Lion Bioscience A.-G., Germany  
 SOURCE: Eur. Pat. Appl., 45 pp.  
 CODEN: EPXQXW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1398029	A1	20040317	EP 2002-20256	20020910
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
WO 2004024148	A1	20040325	WO 2003-EP7066	20030702
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003250877	A1	20040430	AU 2003-250877	20030702
US 2006148876	A1	20060706	US 2005-526940	20051021
PRIORITY APPLN. INFO.:			AT 2002-20256	A 20020910
			WO 2003-EP7066	W 20030702

OTHER SOURCE(S): MARPAT 140:264528  
 AB The invention discloses pyrazole derivs. which bind to the NR3B1 receptor and act as antagonists of the NR3B1 receptor. The invention further relates to the treatment of diseases and/or conditions through binding of the nuclear receptor by the compds., as well as the production of medicaments using the compds.  
 IT 362006-35-7  
 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (NR3B1 nuclear receptor-binding pyrazole derivs., and therapeutic uses)  
 RN 362006-35-7 CAPLUS  
 CN Phenol, 4-[5-(2,5-dimethylphenyl)-1-methyl-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

L11 ANSWER 3 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



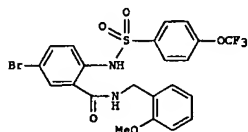
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

current app.

L11 ANSWER 4 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2003:551386 CAPLUS  
 DOCUMENT NUMBER: 139:117209  
 TITLE: Preparation of biaryl phosphate transport inhibitors  
 INVENTOR(S): Jozefiak, Thomas H.; Bastos, Cecilia M.; Papoulias, Andrew T.; Holmes-Farley, Stephen Randall  
 PATENT ASSIGNEE(S): Genzyme Corporation, USA  
 SOURCE: PCT Int. Appl., 135 pp.  
 CODEN: PIXX02  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003057225	A2	20030717	WO 2002-US41481	20021224
WO 2003057225	A3	20040408		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004019113	A1	20040129	US 2002-327627	20021220
US 7119120	B2	20060101		
AU 2002367396	A1	20030724	AU 2002-367396	20021224
EP 1465638	A2	20041013	EP 2002-806234	20021224
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
JP 2005514413	T	20050519	JP 2003-557583	20021224
US 2007021509	A1	20070125	US 2006-489286	20060719
PRIORITY APPLN. INFO.:			US 2001-344660P	P 20011226
			US 2002-371649P	P 20020410
			US 2002-327627	A1 20021220
			WO 2002-US41481	W 20021224

OTHER SOURCE(S): MARPAT 139:117209  
 GI

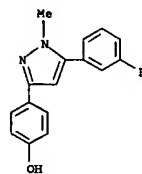


II

AB Disclosed are compds. Ar1-W-X-Y-Ar2 [Ar1-2 = (un)substituted aryl group or 5-6 membered non-aromatic group fused to a (un)substituted monocyclic aryl group; W, Y = covalent bond, alkylene; X = SO2, SO2-alkyl, SO2-amino, etc; I] which are inhibitors of phosphate transport. For instance,

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L11 ANSWER 4 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
 5-bromo-2-[[[4-(trifluoromethoxyphenyl)sulfonyl]amino]benzoic acid (prepn. given) is converted to the acid chloride (SOCl2, reflux) and used to acylate 2-methoxybenzyl amine (THF) to give II. Example compds. inhibit phosphate transport in rabbit intestinal brush border membrane vesicles; a select group of example compds. has IC50 = 0-50 μM. I are used to treat a disease assocd. with hyperphosphatemia, as well as a disease mediated by phosphate-transport function.  
 IT 362016-88-4P  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of biaryl phosphate transport inhibitors)  
 RN 362016-88-4 CAPLUS  
 CN Phenol, 4-[5-(3-fluorophenyl)-1-methyl-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



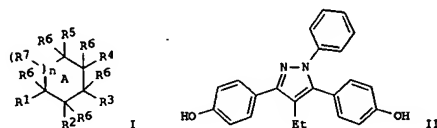
16.44

16.47 = 103

## 10526940claim4

L11 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2000:240935 CAPLUS  
DOCUMENT NUMBER: 132:279214  
TITLE: Preparation of non-steroidal estrogen receptor subtype-selective ligands  
INVENTOR(S): Katzenellenbogen, John A.; Katzenellenbogen, Benita S.; Fink, Brian E.; Stauffer, Shaun R.; Mortensen, Deborah S.; Sattigeri, Viswanathan Jitendra; Huang, Ying  
PATENT ASSIGNEE(S): Board of Trustees of the University of Illinois, USA  
SOURCE: PCT Int. Appl., 134 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

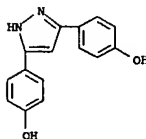
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000019994	A1	20000413	WO 1999-US22747	19991001
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GV, ML, HR, NE, SN, TD, TG				
PRIORITY APPLN. INFO.: MARPAT 132:279214 US 1998-102881P P 19981002				
OTHER SOURCE(S): GI				



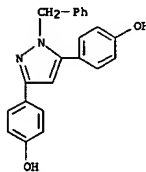
AB Ph substituted pyrazoles, cyclopentadienes, furans, pyrimidines, and their analogs (I) [wherein x = 0 or 1; when x = 0, A = doubly unsatd. 5-membered ring; when x = 1, A = aromatic 6-membered ring; R1 = (un)substituted Ph; R2-R5 and R7 = independently H, basic or polar group, or (un)substituted Ph, alkyl, alkenyl, or alkynyl, or R7 is not present; R6 = H, basic or polar group, or (un)substituted alkyl, alkenyl, alkynyl, or alkoxy; or R6 is not present] were prepared for selective regulation of cellular activity under the control of estrogen receptor (ER) and for the treatment of

L11 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L11 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
hormone-dependent disorders, such as hormone-responsive breast cancer. I have modular structures, which are amenable to solid phase synthesis and the application of combinatorial synthetic methods (no data). I exhibit a spectrum of selective affinities for ERα and ERβ and a spectrum of agonist/antagonist properties. For example, 2-ethyl-1,3-bis(4-methoxyphenyl)-1,3-propanedione was treated with Ph hydrazine.HCl in DMF/THF (89%), followed by BBr3 demethylation in CH2Cl2 to give II (54%). The latter displayed a relatively high ER binding affinity (RBA = 14.0). II also proved to be an ERα potency selective agonist compared to estradiol and showed a 120-fold higher potency in activating transcription via ERα than via ERβ.  
IT 137646-99-2P, 3,5-di(4-hydroxyphenyl)-1H-pyrazole  
234093-03-9P, 1-Benzyl-3,5-di(4-hydroxyphenyl)-1H-pyrazole  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(target compound; preparation of non-steroidal estrogen receptor subtype-selective ligands)  
RN 137646-99-2 CAPLUS  
CN Phenol, 4,4'-(1H-pyrazole-3,5-diyl)bis- (9CI) (CA INDEX NAME)



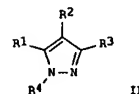
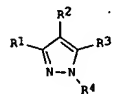
RN 234093-03-9 CAPLUS  
CN Phenol, 4,4'-(1-(phenylmethyl)-1H-pyrazole-3,5-diyl)bis- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 6 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2000:117030 CAPLUS  
DOCUMENT NUMBER: 132:166234  
TITLE: Preparation of estrogen receptor modulating pyrazoles  
INVENTOR(S): Huebner, Verena D.; Lin, Xiaodong; James, Ian; Chen, Liya; Desai, Manoj; Kryvult, Beata; Singh, Rajinder; Wang, Liang  
PATENT ASSIGNEE(S): Chiron Corp., USA  
SOURCE: PCT Int. Appl., 124 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 2  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000007996	A2	19990806	WO 1999-US17799	19990806
WO 2000007996	A3	20000831		
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GV, ML, MR, NE, SN, TD, TG				
AU 9954677	A1	20000228	AU 1999-54677	19990806
EP 1102753	A2	20010530	EP 1999-940917	19990806
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
US 6291505	B1	20010918	US 1999-369747	19990806
JP 2002522422	T	20020723	JP 2000-563630	19990806
US 2002111374	A1	20020815	US 2001-954039	20010918
US 2004034081	A9	20040219		
US 6727273	B2	20040427		
US 2004077701	A1	20040422	US 2003-461914	20030612
PRIORITY APPLN. INFO.: US 1998-95772P P 19980807				
US 1998-95773P P 19980807				
US 1999-369747 A3 19990806				
WO 1999-US17799 W 19990806				
US 2001-954039 A1 20010918				
OTHER SOURCE(S): MARPAT 132:166234				
GI				



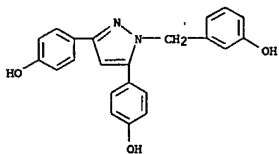
AB The title compds. [I and II; R1, R3 = alkyl, aryl, heteroaryl, etc.; R2 = H, halo, CN, etc.; R4 = H, CO2H, CHO, etc.] which have been found to have unexpected and surprising activity in modulating estrogen receptor activity, and therefore are useful for treating or preventing estrogen

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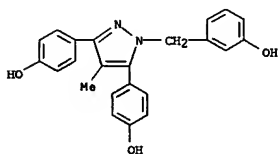
L11 ANSWER 6 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
 receptor-mediated disorders such as osteoporosis, breast and endometrial cancers, atherosclerosis, and Alzheimer's disease, were prepd. E.g., a multi-step synthesis of 11 (R1 = Ph2CH; R2 = Et; R3 = 4-HOCH<sub>2</sub>; R4 = Me), starting with 4'-methoxybutyrylphenone and 2,2-diphenylacetyl chloride, was given (no data for intermediates). Biol. data for compds. I and II were presented.

IT 258847-24-4P 258847-27-7P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of estrogen receptor modulating pyrazoles)

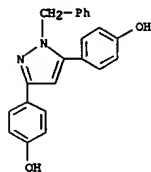
RN 258847-24-4 CAPLUS  
 CN Phenol, 3-[[3,5-bis(4-hydroxyphenyl)-1H-pyrazol-1-yl]methyl]- (9CI) (CA INDEX NAME)



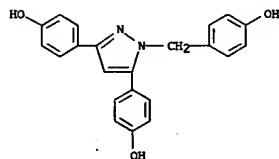
RN 258847-27-7 CAPLUS  
 CN Phenol, 3-[[3,5-bis(4-hydroxyphenyl)-4-methyl-1H-pyrazol-1-yl]methyl]- (9CI) (CA INDEX NAME)



L11 ANSWER 7 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
 CN Phenol, 4,4'-[1-(phenylmethyl)-1H-pyrazole-3,5-diyl]bis- (9CI) (CA INDEX NAME)



RN 234093-04-0 CAPLUS  
 CN Phenol, 4,4'-[1-[(4-hydroxyphenyl)methyl]-1H-pyrazol-3,5-diyl]bis- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 7 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1999:1327909 CAPLUS  
 DOCUMENT NUMBER: 131:125589  
 TITLE: Novel structural templates for estrogen-receptor ligands and prospects for combinatorial synthesis of estrogens

AUTHOR(S): Fink, Brian E.; Mortensen, Deborah S.; Stauffer, Shaun R.; Aron, Zachary D.; Katzenellenbogen, John A.

CORPORATE SOURCE: Department of Chemistry, University of Illinois, Urbana, IL, 61801, USA

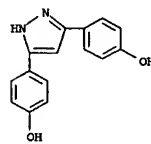
SOURCE: Chemistry & Biology (1999), 6(4), 205-219  
 CODEN: CBOLE2; ISSN: 1074-5521  
 PUBLISHER: Current Biology Publications

DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The development of estrogen pharmaceutical agents with appropriate tissue-selectivity profiles has not yet benefited substantially from the application of combinatorial synthetic approaches to the preparation of structural classes that are known to be ligands for the estrogen receptor (ER). We have developed an estrogen pharmacophore that consists of a simple heterocyclic core scaffold, amenable to construction by combinatorial methods, onto which are appended 3-4 peripheral substituents that embody substructural motifs commonly found in nonsteroidal estrogens. The issue addressed here is whether these heterocyclic core structures can be used to prepare ligands with good affinity for the ER. We prepared representative members of various azole core structures. Although members of the imidazole, thiazole or isoxazole classes generally have weak binding for the ER, several members of the pyrazole class show good binding affinity. The high-affinity pyrazoles bear close conformational relationship to the nonsteroidal ligand raloxifene, and they can be fitted into the ligand-binding pocket of the ER-raloxifene X-ray structure. Compds. such as these pyrazoles, which are novel ER ligands, are well suited for combinatorial synthesis using solid-phase methods.

IT 137646-99-2P 234093-03-9P 234093-04-0P  
 RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)  
 (azoles as structural templates for estrogen-receptor ligands and prospects for combinatorial synthesis of estrogens)

RN 137646-99-2 CAPLUS  
 CN Phenol, 4,4'-[1H-pyrazole-3,5-diyl]bis- (9CI) (CA INDEX NAME)



RN 234093-03-9 CAPLUS

L11 ANSWER 8 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1997:86817 CAPLUS  
 DOCUMENT NUMBER: 126:179299  
 TITLE: FLCs with a five-membered ring in the mesogenic core

AUTHOR(S): Iglesias, R.; Serrano, J. L.; Sierra, T.

CORPORATE SOURCE: Fac. Cienc.-Inst. Cienc. Mater. Aragon, Univ. Zaragoza, Zaragoza, 50009, Spain

SOURCE: Liquid Crystals (1997), 22(1), 37-46  
 CODEN: LICRE6; ISSN: 0267-8292

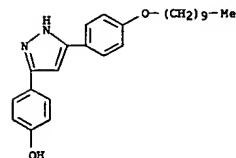
PUBLISHER: Taylor & Francis  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB A study was undertaken of the structure-activity relation of eight new chiral compds. having either a pyrazole or an isoxazole ring as a central bridge in the mesogenic core. The presence of dimers in the pyrazole compds. accounts for their lower P<sub>s</sub> values in comparison with the isoxazole analogs. The corresponding four β-diketone precursors also were studied and these, as expected given their bent mol. shape, show much worse mesomorphic and ferroelec. behavior. To complete the study, the mol. dipoles of the three types of derivative were determined using AM1 calcns.

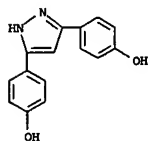
Two types of chiral tail were incorporated into the compds.: alkoxy and alkanoyloxy. The latter tail gives rise to the best mesomorphic and ferroelec. properties. A study of the tail conformation by MM2 calcns. provides an explanation of these results. The highest P<sub>s</sub> value (137 nC cm<sup>-2</sup>) was obtained for the isoxazole derivative with the (2S)-2-butylxypropanoyloxy chiral tail. The potential of all twelve compds. as chiral dopants for FLC mixts. was evaluated by a study of 10 mol.% binary mixts. in a standard host system.

IT 187334-75-4P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and reaction with Bu lactate)

RN 187334-75-4 CAPLUS  
 CN Phenol, 4-[5-[4-(decyloxy)phenyl]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

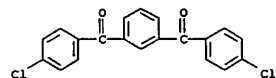


L11 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1996:614968 CAPLUS  
 DOCUMENT NUMBER: 125:248658  
 TITLE: Synthesis and properties of poly(arylene ether pyrazole)s  
 AUTHOR(S): Srinivasan, K. R.; Bass, R. G.; Smith, J. G.  
 CORPORATE SOURCE: Dep. Chem., Virginia Commonwealth Univ., Richmond, VA, 23284-2006, USA  
 SOURCE: High Performance Polymers (1996), 8(3), 381-393  
 CODEN: HPPPOX; ISSN: 0954-0083  
 PUBLISHER: Institute of Physics Publishing  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Poly(arylene ether pyrazole)s containing NH and NPh groups were prepared by the aromatic nucleophilic displacement reaction of two new bisphenols containing a pyrazole ring with activated aromatic dihalides in N,N-dimethylacetamide at 155° in the presence of anhydrous potassium carbonate. The polymers exhibited glass transition temps. (T<sub>g</sub>) ranging from 190-296° and inherent viscosities from 0.44-1.96 dL g<sup>-1</sup>. Poly(arylene ether-pyrazole)s containing NH groups exhibited higher T<sub>g</sub> and mech. properties than the corresponding N-phenyl-containing poly(arylene ether pyrazole)s. The chemical, phys. and mech. properties of these polymers are discussed.  
 IT 137646-99-2P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (monomer for synthesis of bis(hydroxyphenyl)pyrazoles)  
 RN 137646-99-2 CAPLUS  
 CN Phenol, 4,4'-(1H-pyrazole-3,5-diyl)bis- (9CI) (CA INDEX NAME)

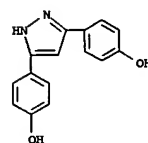


IT 137647-00-8P 137647-01-9P 137661-49-5P  
 182233-43-8P 182233-58-5P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (synthesis and properties of poly(arylene ether pyrazoles))  
 RN 137647-00-8 CAPLUS  
 CN Phenol, 4,4'-(1H-pyrazole-3,5-diyl)bis-, polymer with 1,1'-sulfonylbis[4-chlorobenzene] (9CI) (CA INDEX NAME)  
 CM 1  
 CRN 137646-99-2

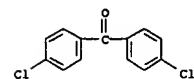
L11 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
 CMF C20 H12 Cl2 O2



RN 137661-49-5 CAPLUS  
 CN Methanone, bis(4-chlorophenyl)-, polymer with 4,4'-(1H-pyrazole-3,5-diyl)bis[phenol] (9CI) (CA INDEX NAME)  
 CM 1  
 CRN 137646-99-2  
 CMF C15 H12 N2 O2

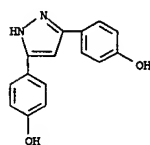


CM 2  
 CRN 90-98-2  
 CMF C13 H8 Cl2 O

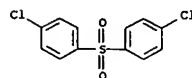


RN 182233-43-8 CAPLUS  
 CN Methanone, 1,4-phenylenebis[(4-fluorophenyl)-, polymer with 4,4'-(1H-pyrazole-3,5-diyl)bis[phenol] (9CI) (CA INDEX NAME)  
 CM 1  
 CRN 137646-99-2  
 CMF C15 H12 N2 O2

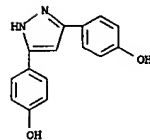
L11 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
 CMF C15 H12 N2 O2



CM 2  
 CRN 80-07-9  
 CMF C12 H8 Cl2 O2 5

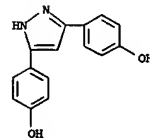


RN 137647-01-9 CAPLUS  
 CN Methanone, 1,3-phenylenebis[(4-chlorophenyl)-, polymer with 4,4'-(1H-pyrazole-3,5-diyl)bis[phenol] (9CI) (CA INDEX NAME)  
 CM 1  
 CRN 137646-99-2  
 CMF C15 H12 N2 O2

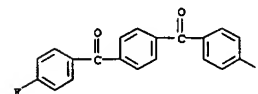


CM 2  
 CRN 22198-44-3

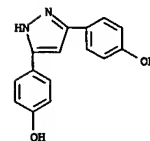
L11 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2  
 CRN 68418-51-9  
 CMF C20 H12 F2 O2

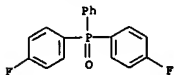


RN 182233-58-5 CAPLUS  
 CN Phenol, 4,4'-(1H-pyrazole-3,5-diyl)bis-, polymer with bis(4-fluorophenyl)phenylphosphine oxide (9CI) (CA INDEX NAME)  
 CM 1  
 CRN 137646-99-2  
 CMF C15 H12 N2 O2



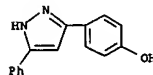
CM 2  
 CRN 54300-32-2  
 CMF C18 H13 F2 O P

L11 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

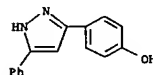


L11 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1994:639383 CAPLUS  
 DOCUMENT NUMBER: 121:239383  
 TITLE: Stability constants of iron(III), chromium(III) and aluminum(III) chelates with some substituted pyrazoles  
 AUTHOR(S): Sawalakhe, P. D.; Narwade, M. L.; Wadodkar, K. N.  
 CORPORATE SOURCE: Department of Chemistry, Vidarbha Mahavidyalaya, Amravati, 444 604, India  
 SOURCE: Journal of the Indian Chemical Society (1994), 71(1), 49-51  
 CODEN: JICSAH; ISSN: 0019-4522  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The interactions of Fe<sup>3+</sup>, Cr<sup>3+</sup> and Al<sup>3+</sup> metal ions with 3-(2-hydroxyphenyl)-5-phenylpyrazole, 3-(2-hydroxy-5-methylphenyl)-5-phenylpyrazole and 3-(2-hydroxy-5-methylphenyl)-5-(4-methoxyphenyl)pyrazole have been investigated potentiometrically in 70% dioxane-water mixture as a solvent at 0.1 M ionic strength. The proton-ligand and metal-ligand stability consts. were determined  
 IT 75059-29-9  
 RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent) (ionization constant of)  
 RN 75059-29-9 CAPLUS  
 CN Phenol, 4-(5-phenyl-1H-pyrazol-3-yl)- (9CI) (CA INDEX NAME)



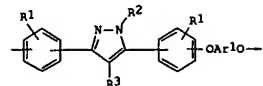
IT 75059-29-9D, transition metal complexes  
 RL: PMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)  
 (stability constant of)  
 RN 75059-29-9 CAPLUS  
 CN Phenol, 4-(5-phenyl-1H-pyrazol-3-yl)- (9CI) (CA INDEX NAME)



L11 ANSWER 11 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN

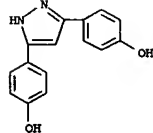
ACCESSION NUMBER: 1994:135439 CAPLUS  
 DOCUMENT NUMBER: 120:135439  
 TITLE: Aromatic polyethers containing pyrazole units and monomers for their preparation  
 INVENTOR(S): Pfendner, Rudolf; Wolf, Jean Pierre; Kainmueller, Thomas; Kramer, Andreas; Hoffmann, Kurt; Stockinger, Friedrich  
 PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.  
 SOURCE: Ger. Offen., 17 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4230839	A1	19930325	DE 1992-4230839	19920915
PRIORITY APPLN. INFO.:			CH 1991-2753	A 19910918

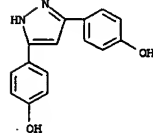


AB Polyethers with good thermal stability and solubility in organic solvents contain  
 1-100 mol% segments I (R1, R3 = alkyl, alkoxy, aryl, aryloxy, halogen; R2 = H, alkyl, Ph; Ar1 = dihalogenated arylene activated for nucleophilic exchange) and 99-0 mol% segments -OAr2OAr1- (Ar2 = arylene). Treatment of Et 4-methoxybenzoate with NaH and then condensation with 4-methoxyacetophenone in glyme gave 68% 1,3-bis(4-methoxyphenyl)-1,3-propanedione, cyclization of which with NH4.H2O gave 42% 3,5-bis(4-methoxyphenyl)pyrazole, which was demethylated by CSH5N.HCl in 61% yield to the bisphenol (II). Heating II 0.0501, 4,4'-sulfonyldiphenol 0.1562, (4-ClC6H4)2SO2 0.2001, and K2CO3 0.2116 mol for 6 h at 225-280° gave a polyether with reduced viscosity 0.45 dL/g, glass temperature 223°, decomposition temperature (TGA) 510°, and solubility in N-methylpyrrolidone and CH2Cl2 >25%.  
 IT 137646-99-2P, 4,4'-(3,5-Pyrazolediyl)diphenol  
 RL: PREP (Preparation)  
 (preparation of)  
 RN 137646-99-2 CAPLUS  
 CN Phenol, 4,4'-(1H-pyrazole-3,5-diyl)bis- (9CI) (CA INDEX NAME)

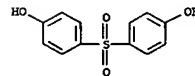
L11 ANSWER 11 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



IT 151485-79-9P  
 RL: PREP (Preparation)  
 (preparation of heat-resistant, with good solubility)  
 RN 151485-79-9 CAPLUS  
 CN Phenol, 4,4'-(1H-pyrazole-3,5-diyl)bis-, polymer with 1,1'-sulfonylbis[4-chlorobenzene] and 4,4'-sulfonylbis[phenol] (9CI) (CA INDEX NAME)  
 CH 1  
 CRN 137646-99-2  
 CMF C15 H12 N2 O2

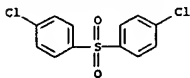


CH 2  
 CRN 80-09-1  
 CMF C12 H10 O4 S



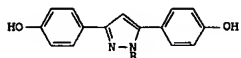
CH 3  
 CRN 80-07-9  
 CMF C12 H8 C12 O2 S

L11 ANSWER 11 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L11 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN

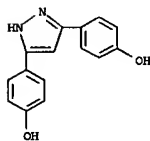
ACCESSION NUMBER: 1991:680692 CAPLUS  
 DOCUMENT NUMBER: 115:280692  
 TITLE: Synthesis of poly(arylene ether pyrazoles) by aromatic nucleophilic displacement reactions  
 AUTHOR(S): Bass, R. G.; Srinivasan, K. R.  
 CORPORATE SOURCE: Dep. Chem., Virginia Commonw. Univ., Richmond, VA, 23284-2006, USA  
 SOURCE: Polymer Preprints (American Chemical Society, Division of Polymer Chemistry) (1991), 32(1), 619-20  
 CODEN: ACPPAY; ISSN: 0032-3934  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB Title polyethers were prepared by the condensation of bisphenols I (R = H, Ph) with dihalides 4-R1C6H4XC6H4R1-4 (R1 = Cl, F; X = CO, SO2, isophthaloyl, terephthaloyl, 4-COC6H4OC6H4CO-4).  
 IT 137647-00-8P 137647-01-9P 137647-02-0P  
 137661-49-5P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and properties of)  
 RN 137647-00-8 CAPLUS  
 CN Phenol, 4,4'-(1H-pyrazole-3,5-diyl)bis-, polymer with 1,1'-sulfonylbis[4-chlorobenzene] (9CI) (CA INDEX NAME)

CH 1

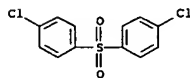
CRN 137646-99-2  
 CHF C15 H12 N2 O2



CH 2

L11 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

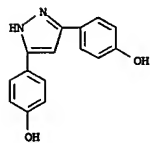
CRN 80-07-9  
 CMF C12 H8 Cl2 O2 S



RN 137647-01-9 CAPLUS  
 CN Methanone, 1,3-phenylenebis[(4-chlorophenyl)-, polymer with 4,4'-(1H-pyrazole-3,5-diyl)bis[phenol] (9CI) (CA INDEX NAME)

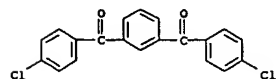
CH 1

CRN 137646-99-2  
 CMF C15 H12 N2 O2



CH 2

CRN 22198-44-3  
 CMF C20 H12 Cl2 O2

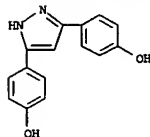


RN 137647-02-0 CAPLUS  
 CN Methanone, 1,4-phenylenebis[(4-chlorophenyl)-, polymer with 4,4'-(1H-pyrazole-3,5-diyl)bis[phenol] (9CI) (CA INDEX NAME)

CH 1

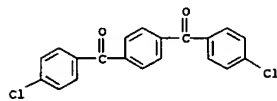
CRN 137646-99-2  
 CMF C15 H12 N2 O2

L11 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CH 2

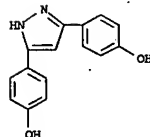
CRN 22198-42-1  
 CMF C20 H12 Cl2 O2



RN 137661-49-5 CAPLUS  
 CN Methanone, bis(4-chlorophenyl)-, polymer with 4,4'-(1H-pyrazole-3,5-diyl)bis[phenol] (9CI) (CA INDEX NAME)

CH 1

CRN 137646-99-2  
 CMF C15 H12 N2 O2

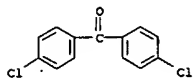


CH 2

CRN 90-98-2  
 CMF C13 H8 Cl2 O

10526940claim4

L11 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L11 ANSWER 13 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1980:567052 CAPLUS  
DOCUMENT NUMBER: 93:167052  
TITLE: Luminescence properties of arylpyrazoles  
AUTHOR(S): Udachin, Yu. M.; Chursinova, L. V.; Przheval'skii, N. M.; Grandberg, I. I.; Tokmakov, G. P.  
CORPORATE SOURCE: Mosk. S-kh. Akad., Moscow, USSR  
SOURCE: Izvestiya Timiryazevskoi Sel'skokhozyaistvennoi Akademii (1980), (3), 162-9  
CODEN: ITSAA7; ISSN: 0021-342X

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB The absorption and emission spectra and luminescence quantum yields of mono-, di-, and triarylpyrazoles were determined in different solvents and

at liquid N and room temperature. Steric effects played a major role, e.g., 1,5-diarylpyrazoles exhibited absorption maximum at shorter wavelengths than 1,3- or 1,4-diarylpyrazoles owing to aryl ring interaction, which decreased the coplanarity of the mol. Triarylpyrazoles showed severe fluorescence quenching for the same reason. Calcn. of the charge distribution in the ground (S0) and excited singlet (S1) states of 1,3-diphenylpyrazole indicated that excitation was accompanied by transfer of electron d. from N-1, C-3, and the 3-Ph ring to N-2.

IT 75059-29-9

RL: PRP (Properties)

(absorption and fluorescence spectra of)

RN 75059-29-9 CAPLUS

CN Phenol, 4-(5-phenyl-1H-pyrazol-3-yl)- (9CI) (CA INDEX NAME)

